

Introduction of Computational Fluid Dynamics

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1. Basics of Computational Fluid Dynamics

1.1. Concept of Computational Fluid Dynamics

Computational Fluid Dynamics (CFD) is the simulation of fluids engineering systems using modeling (mathematical physical problem formulation) and numerical methods (discretization methods, solvers, numerical parameters, and grid generations, etc.). The process is as figure 1.

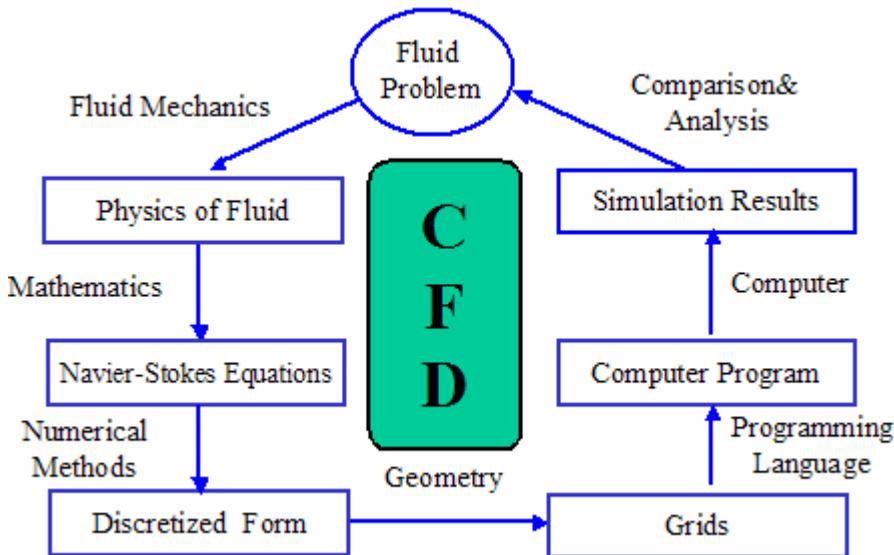


Figure 1 Process of Computational Fluid Dynamics

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 and it is the governing equation of CFD. As 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,

Finite Volume 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. Normally the programs are run on workstations or supercomputers. At the end, we can get our simulation results. We can compare and analyze the simulation results with experiments and 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 the process of CFD.

1.2. Importance of Computational Fluid Dynamics

There are three methods in study of Fluid: theory analysis, experiment and simulation (CFD). As a new method, CFD has many advantages compared to experiments. Please refer table 1.

	Simulation (CFD)	Experiment
Cost	Cheap	Expensive
Time	Short	Long
Scale	Any	Small/Middle
Information	All	Measured Point
Repeatable	Yes	Some
Safety	Yes	Some Dangerous

Table 1 Comparison of Simulation and Experiment

1.3. Application of Computational Fluid Dynamics

As CFD has so many advantages, it is already generally used in industry such as aerospace, automotive, biomedicine, chemical processing, heat ventilation air condition, hydraulics, power generation, sports and marine etc.

1.4. Physics of Fluid

Fluid is liquid and gas. For example, water and air. Fluid has many important properties, such as velocity, pressure, temperature, density and viscosity.

The density (1) of a fluid is its mass per unit volume. If the density of fluid is constant (or the change is very small), we call the fluid is incompressible fluid. If the density of fluid is not constant, we call the fluid is compressible fluid. Normally, we can treat water and air as incompressible fluid. If the fluid is incompressible, we can simplify the equations for this type of fluid.

$$\rho = \frac{M}{V} \left[\frac{\text{kg}}{\text{m}^3} \right] \quad (1)$$

The viscosity (2) is an internal property of a fluid that offers resistance to flow. For example, to stir water is much easier than to stir honey because the viscosity of water is much smaller than honey.

$$\mu = \left[\frac{Ns}{m^3} \right] = [Posie] \quad (2)$$

Table 2 shows the densities and viscosities 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

2. 2. Navier-Stokes Equations

2.1. Conservation Law

Navier-Stokes equations are the governing equations of Computational Fluid Dynamics. It is based on the conservation law of physical properties of fluid. The principle of conservational law is the change of properties, for example mass, energy, and momentum, in an object is decided by the input and output.

For example, the change of mass in the object is as follows

$$\frac{dM}{dt} = \dot{m}_{in} - \dot{m}_{out} \quad (3)$$

If $\dot{m}_{in} - \dot{m}_{out} = 0$, we have

$$\frac{dM}{dt} = 0 \quad (4)$$

Which means

$$M = const \quad (5)$$

2.2. Navier-Stokes Equation

Applying the mass, momentum and energy conservation, we can derive the continuity equation, momentum equation and energy equation as follows.

Continuity Equation

$$\frac{D\rho}{Dt} + \rho \frac{\partial U_i}{\partial x_i} = 0 \quad (7)$$

Momentum Equation

$$\underbrace{\rho \frac{\partial U_j}{\partial t}}_I + \underbrace{\rho U_i \frac{\partial U_j}{\partial x_i}}_{II} = - \underbrace{\frac{\partial P}{\partial x_j}}_{III} - \underbrace{\frac{\partial \tau_{ij}}{\partial x_i}}_{IV} + \underbrace{\rho g_j}_V \quad (8)$$

Where

$$\tau_{ij} = -\mu \left(\frac{\partial U_j}{\partial x_i} + \frac{\partial U_i}{\partial x_j} \right) + \frac{2}{3} \delta_{ij} \mu \frac{\partial U_k}{\partial x_k} \quad (9)$$

- I: Local change with time
- II: Momentum convection
- III: Surface force
- IV: Molecular-dependent momentum exchange (diffusion)
- V: Mass force

Energy Equation

$$\underbrace{\rho c_\mu \frac{\partial T}{\partial t}}_I + \underbrace{\rho c_\mu U_i \frac{\partial T}{\partial x_i}}_{II} = -P \underbrace{\frac{\partial U_i}{\partial x_i}}_{III} + \lambda \underbrace{\frac{\partial^2 T}{\partial x_i^2}}_{IV} - \underbrace{\tau_{ij} \frac{\partial U_j}{\partial x_i}}_V \quad (10)$$

- I : Local energy change with time
- II: Convective term
- III: Pressure work
- IV: Heat flux (diffusion)
- V: Irreversible transfer of mechanical energy into heat

If the fluid is compressible, we can simplify the continuity equation and momentum equation as follows.

Continuity Equation

$$\frac{\partial U_i}{\partial x_i} = 0 \quad (11)$$

Momentum Equation

$$\rho \frac{\partial U_j}{\partial t} + \rho U_i \frac{\partial U_j}{\partial x_i} = - \frac{\partial P}{\partial x_j} - \mu \frac{\partial^2 U_j}{\partial x_i^2} + \rho g_j \quad (12)$$

2.3. General Form of Navier-Stokes Equation

To simplify the Navier-Stokes equations, we can rewrite them as the general form.

$$\frac{\partial(\rho\Phi)}{\partial t} + \frac{\partial}{\partial x_i} \left(\rho U_i \Phi - \Gamma_\Phi \frac{\partial \Phi}{\partial x_i} \right) = q_\Phi \quad (13)$$

When $\Phi = 1, U_j, T$, we can respectively get continuity equation, momentum equation and energy equation.

3. Finite Volume Method

The Navier-Stokes equations are analytical equations. Human can understand and solve them, but if we want to solve them by computer, we have to transfer them into discretized form. This process is discretization. The typical discretization methods are finite difference, finite element and finite volume methods. Here we introduce finite volume method.

3.1. The Approach of Finite Volume Method

Integrate the general form of Navier-Stokes equation over a control volume and apply Gauss Theory

$$\int_V \frac{\partial}{\partial x_i} \Phi dV = \int_S \Phi \cdot n_i dS \quad (14)$$

We can get the integral form of Navier-Stoke equation

$$\int_V \frac{\partial(\rho\Phi)}{\partial t} dV + \int_S \left(\rho U_i \Phi - \Gamma \frac{\partial \Phi}{\partial x_i} \right) \cdot n_i dS = \int_V q_\Phi dV \quad (15)$$

To approximate the the volume integral, we can multiply the volume and the value at the center of the control volume. For example, we have a 2D domain as fig 2. To approximate the mass and momentum of control volume P, we have

$$m = \int_{V_i} \rho dV \approx \rho_p V, \quad mu = \int_{V_i} \rho_i u_i dV \approx \rho_p u_p V \quad (16)$$

To approximate the surface integral, for example pressure force, we have

$$\oint_{S_i} P dS \approx \sum_k P_k S_k \quad k = n, s, e, w \quad (17)$$

Normally we store our variables at the center of control volume, so we need to interpolate them to get P_k , which are located at the surface of control volume.

Typically, we have two types of interpolations, one is upwind interpolation, and the other one is central interpolation.

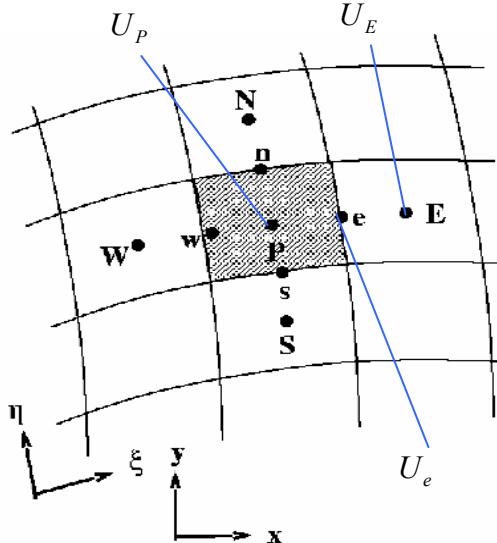


Figure 2 2D Structured Grid Domain

Upwind Interpolation

$$U_e = \begin{cases} U_P & \text{if } (\vec{U} \cdot \vec{n})_e > 0 \\ U_E & \text{if } (\vec{U} \cdot \vec{n})_e < 0 \end{cases}$$

Central Interpolation

$$U_e = U_E \lambda_e + U_P (1 - \lambda_e) \quad \lambda_e = \frac{x_e - x_P}{x_E - x_P}$$

3.2. Conservation of Finite Volume Method

If we use finite difference and finite element approach to discretized Navier-Stokes equation, we have to manually control the conservation of mass, momentum and energy. But with finite volume method, we can easily find out that, if the Navier-Stokes equation is satisfied in every control volume, it will automatically be satisfied for the whole domain. In another words, if the conservation is satisfied in every control volume, it will be automatically satisfied in whole domain.

That is the reason why finite volume is preferred in computational fluid dynamics.

4. Grids

There are three types of grids: structured grids, unstructured grids and block structured grids.

The simplest one is structured grid (fig 3). 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. For example, fig 4 is an airfoil. The structure of airfoil is very complex. The flow near the object is very important and complex, we need very fine grid at this region. Far away from the airfoil, the flow is comparably simple, so we can use coarse 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, then use different structured grids in different blocks.

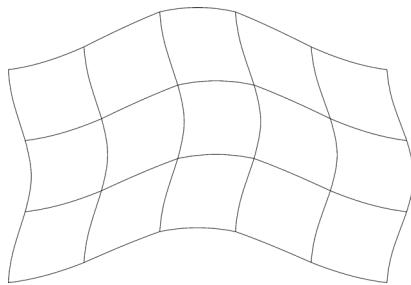


Figure 3 Structured Grids

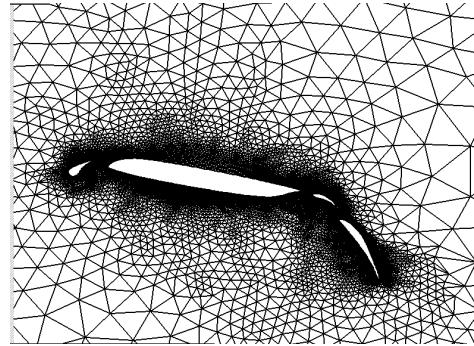


Figure 4 Unstructured Grids

5. 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, fig 5 is a pipe, the fluid flows from left to right. We can use inlet at left side, which means we can set the velocity manually. At the right side, we use outlet boundary condition to keep all the properties constant, which means all the gradients are zero.

At the wall of pipe, we can set the velocity to zero. This is no-slip boundary condition.

At the center of pipe, we can use axisymmetric boundary condition.

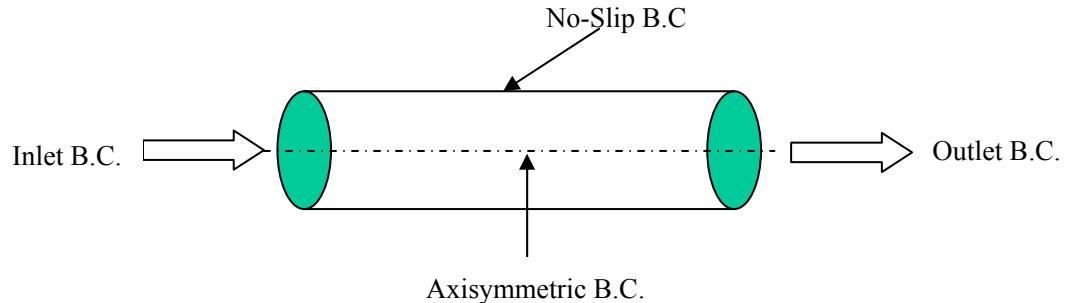


Figure 5 Boundary Conditions of Pipe Flow