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Systematic computational methods of unsteady flow simulation based on computational fluid dynamics

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Abstract. Unsteady flow is the dominant flow state in real life; thus, the simulation of it is of vital importance, especially in engineering, for example, the flutter or buffeting of the aerofoil. In the past decades, the progress in computational science greatly paced the development of computational fluid dynamics (CFD), providing powerful tools for simulating unsteady flow via numerical methods. However, the unsteady flow state depends on more variables than a steady flow, including the external conditions in different time moments and the flow's properties that vary with time. The calculation is still too massive, even using CFD. Therefore, CFD algorithms with higher efficiency and less reduction in accuracy are still needed to optimize the technique. This paper reviews the main CFD computational methods that have been maturely developed and proven effective, including direct numerical simulation (DNS), classic turbulence models and reduced order model (ROM), illustrating the main mechanisms and displaying their features. The paper also sheds light on these methods' latest research progress.

Keywords: computational fluid dynamics, numerical methods, unsteady flow simulation.

1. Introduction

Unsteady flow is the most common flow state in the natural world and practical engineering. The main causes for unsteadiness are unsteady boundary conditions and flow instability, while the variation of external forces and energy contributes [1]. Compared with a steady flow, the behaviors of flow or fluid micelles depend not only on the current flow state and boundary condition but also on the flow states in former moments, including the external conditions and the state variables, which is more complicated and requires more calculation resources. The research methods of unsteady flow include theoretical models, numerical simulation and wind tunnel test [2]. While the theoretical model strongly relies on linear assumptions, which restricts its accuracy and application, and wind tunnel test requires high cost and cumbersome operations, numerical simulation, often carried out through computational fluid dynamics (CFD) thanks to advances in computational science, becomes the main approach to study and predict the behaviors of a fluid field. However, direct numerical methods often require plenty of computational resources and data storage capacity, while unsteady flow adds an extra dimension and lowers calculation efficiency. Besides, unknown phase and integration errors can cause serious instability when predicting the behavior and even lead to incorrections [3]. Furthermore, approximations are usually introduced to model the deforming fluid–structure boundary, which may violate the required consistency or conformity conditions between the fluid and solid elements and

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cause incorrect modeling [4]. Therefore, more efficient and precise models must be developed to facilitate CFD in unsteady flow simulations. This paper presents the main calculational approaches in CFD that have been maturely applied and updates the research process and new appliance of the methods. In the paper, φ stands for a general fluid field variable, for example, velocity, potential or temperature, and the variables in bold represent vectors or matrixes.

Generally, all the numerical methods are based on one or several governing equations, which illustrate the core laws to which the flow conforms. N-S equations are the essential ones that apply to a wide range of flow types. Based on the conservation laws of mass, momentum and energy, N-S equations can be expressed in an integral form:

$$\frac{\partial}{\partial t}\iiint_{\Omega}\boldsymbol{U}dV+\iint_{\partial\Omega}\boldsymbol{F}(\boldsymbol{U})\cdot\boldsymbol{n}dS+\iint_{\partial\Omega}\boldsymbol{G}(\boldsymbol{U})\cdot\boldsymbol{n}dS=0$$

$$\boldsymbol{U}=\begin{bmatrix}\rho\\ \rho u_x\\ \rho u_y\\ \rho u_z\\ e_0\end{bmatrix},\boldsymbol{F}(\boldsymbol{U})\cdot\boldsymbol{n}=\begin{bmatrix}\rho\\ \rho u_x+Pn_x\\ \rho u_y+Pn_y\\ \rho u_z+Pn_z\\ e_0+P\end{bmatrix},\boldsymbol{G}(\boldsymbol{U})\cdot\boldsymbol{n}=\frac{M_\infty}{Re}\left(n_x\boldsymbol{G}_1+n_y\boldsymbol{G}_2+n_z\boldsymbol{G}_3\right)$$

$$\boldsymbol{G}_1=\begin{bmatrix}0\\ \tau_{xx}\\ \tau_{xy}\\ \tau_{xz}\\ u_x\tau_{xx}+u_y\tau_{xy}+u_z\tau_{xz}+k\dfrac{\partial T}{\partial x}\end{bmatrix},\ \boldsymbol{G}_2=\begin{bmatrix}0\\ \tau_{yx}\\ \tau_{yy}\\ \tau_{yz}\\ u_x\tau_{yx}+u_y\tau_{yy}+u_z\tau_{yz}+k\dfrac{\partial T}{\partial y}\end{bmatrix},$$

$$\boldsymbol{G}_3=\begin{bmatrix}0\\ \tau_{zx}\\ \tau_{zy}\\ \tau_{zz}\\ u_x\tau_{zx}+u_y\tau_{zy}+u_z\tau_{zz}+k\dfrac{\partial T}{\partial z}\end{bmatrix},\tau_{ij}=\mu\left(\partial_i u_j+\partial_j u_i\right)-\frac{2}{3}\mu\cdot div(\boldsymbol{u})\delta_{ij}$$

where ρ is the density of the fluid, $\boldsymbol{u}=\left(u_x,u_y,u_z\right)^T$ is the velocity of the mass point, $\boldsymbol{n}=\left(n_x,n_y,n_z\right)^T$ is the normal vector of the fluid at the point, P is the fluid pressure, e_0 is the total fluid internal energy, τ_{ij} is the stress article, k is the heat conduction coefficient, T is the fluid temperature, and μ is the kinematic coefficient of viscosity. The equations apply to continuous medium and Newton fluid at normal pressure and temperature without body forces considered. On account of that, there are Euler equations for inviscid fluids:

$$\frac{\partial}{\partial t}\iiint_{\Omega}\boldsymbol{U}dV+\iint_{\partial\Omega}\boldsymbol{F}(\boldsymbol{U})\cdot\boldsymbol{n}dS=0$$

And full potential equations for irrotational, isentropic flow are also widely used to simulate their solutions in certain conditions:

$$\frac{1}{c^2}\left[\phi_{tt}+\partial_t\left(\left|\nabla\phi\right|^2\right)\right]=\left(1-M_x^2\right)\phi_{xx}+\left(1-M_y^2\right)\phi_{yy}+\left(1-M_z^2\right)\phi_{zz}-2M_xM_y\phi_{xy}-2M_yM_z\phi_{yz}$$
$$-2M_zM_x\phi_{zx}$$

$$c^2=(\gamma-1)\left[H_0-\frac{1}{2}\left|\nabla\phi\right|^2-\phi_t\right],\ \nabla\phi=u_x\boldsymbol{i}+u_y\boldsymbol{j}+u_z\boldsymbol{k}$$

where ϕ represents potential, c is the sound velocity, H_0 is the stagnation enthalpy, γ is the ratio of specific heat and M_x, M_y, M_z are the Mach numbers in the three directions.

2. Direct numerical simulation (DNS)

With the governing equations established in the last chapter, most of which are in complex ODE or PDE forms and cannot be solved analytically, CFD provides a tool to simulate their numerical

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solutions, so the main task of DNS is to give the solutions. Two parts of the work are discussed here, including spatial discretization and time discretization. Three spatial discretization methods are introduced, including finite difference method (FDM), finite volume method (FVM) and finite element method (FEM) and the time discretization methods are displayed in three types: time domain marching method, frequency domain harmonic method and time domain collocation method [1]. As the two discretization aspects are displayed individually, only steady flows are discussed in the spatial discretization part, for unsteady flow can be seen as steady at every unit time interval.

2.1. Spatial discretization

2.1.1. FDM. FDM is a classic method for solving differential equations numerically, simply and straightforwardly. It subdivides the definitional domain into meshes, with the information of functions preserved in nodes and derivatives expressed with difference quotients. Consider a 2D scalar function $\varphi_{i,j} = \varphi(x, y)$, with i representing the mesh node in x direction and j representing that in y direction, it is similar for 3D circumstances. Express φ with the Taylor series:

$$\begin{cases} \varphi_{i+1,j} = \varphi_{i,j} + \frac{\partial \varphi}{\partial x}|_{i,j} \cdot \Delta x + \frac{\partial^2 \varphi}{\partial x^2}|_{i,j} \cdot \Delta x^2 + \dots \\ \varphi_{i-1,j} = \varphi_{i,j} - \frac{\partial \varphi}{\partial x}|_{i,j} \cdot \Delta x + \frac{\partial^2 \varphi}{\partial x^2}|_{i,j} \cdot \Delta x^2 - \dots \end{cases} \tag{1}$$

and it is also true for $\varphi_{i,j+1}$ and $\varphi_{i,j-1}$. It's easy to derive the following relationships with the Taylor series:

$$\begin{cases} \frac{\partial \varphi}{\partial x} = \frac{\varphi_{i+1,j} - \varphi_{i,j}}{\Delta x} + O(\Delta x) \\ \frac{\partial \varphi}{\partial x} = \frac{\varphi_{i,j} - \varphi_{i-1,j}}{\Delta x} + O(\Delta x) \\ \frac{\partial \varphi}{\partial x} = \frac{\varphi_{i+1,j} - \varphi_{i-1,j}}{2\Delta x} + O(\Delta x^2) \end{cases} \tag{2}$$

$$\frac{\partial^2 \varphi}{\partial x^2} = \frac{\varphi_{i+1,j} - 2\varphi_{i,j} + \varphi_{i-1,j}}{\Delta x^2} + O(\Delta x^2) \tag{3}$$

$$\frac{\partial^2 \varphi}{\partial x \partial y} = \frac{\varphi_{i+1,j+1} - \varphi_{i+1,j-1} - \varphi_{i-1,j+1} + \varphi_{i-1,j-1}}{4\Delta x \Delta y} + O(\Delta x^2, \Delta y^2) \tag{4}$$

Theoretically, any order of derivative can be expressed in any order of accuracy using different numbers of nodes, making the accuracy of the general simulation vary. Plug the derivatives into the differential equations using the known boundary conditions, and the value of function u can be solved at every time step. However, the meshes in FDM should be chosen carefully, as some FDM schemes may lead to unstable solutions with overlarge step sizes. Even though some iteration methods, including successive over relaxation (SOR), were introduced to accelerate convergence, FDM still reveals too much unstableness and restrictions in complex circumstances.

2.1.2. FVM. Instead of differential equations used in FDM, FVM is based on the conservation laws in each control volume. For a 3D conservation equation in a general form:

$$div(\rho u \varphi) = \frac{\partial}{\partial x}\left(\Gamma \frac{\partial \varphi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\Gamma \frac{\partial \varphi}{\partial y}\right) + \frac{\partial}{\partial z}\left(\Gamma \frac{\partial \varphi}{\partial z}\right) + S \tag{5}$$

where $div(\rho u \varphi)$ is a convective term, Γ is the diffusion coefficient, and S is the source term. Do an integration with the equation in control volumes and apply the Gauss divergence theorem:

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$$\int_{CV} div(\rho u\varphi) = \int_{CV} \frac{\partial}{\partial x}\left(\Gamma \frac{\partial \varphi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\Gamma \frac{\partial \varphi}{\partial y}\right) + \frac{\partial}{\partial z}\left(\Gamma \frac{\partial \varphi}{\partial z}\right) + \int_{CV} S \tag{6}$$

$$[(\rho u\varphi)_e - (\rho u\varphi)_w] + [(\rho u\varphi)_n - (\rho u\varphi)_s] + [(\rho u\varphi)_o - (\rho u\varphi)_i] = \bar{S}\Delta V + [\left(\Gamma A \frac{\partial \varphi}{\partial x}\right)_e -$$

$$\left(\Gamma A \frac{\partial \varphi}{\partial x}\right)_w] + [\left(\Gamma A \frac{\partial \varphi}{\partial y}\right)_n - \left(\Gamma A \frac{\partial \varphi}{\partial y}\right)_s] + [\left(\Gamma A \frac{\partial \varphi}{\partial z}\right)_o - \left(\Gamma A \frac{\partial \varphi}{\partial z}\right)_i] \tag{7}$$

where A is the area at the boundary of the control volume and e, w, n, s, o, i are respectively short for east, west, north, south, out and in, which indicate the direction of six different directions around the central point of control volume P. As S can be expressed as the sum of a constant and a variable of φ:

$$S = S_c + S_P\varphi_P$$

And φ, as well as its derivatives, can be approximated by the value at P (take x direction as an example) and boundaries of the control volume:

$$(\rho u\varphi)_e - (\rho u\varphi)_w = (\rho u)_e A_e \frac{\varphi_P + \varphi_E}{2} - (\rho u)_w A_w \frac{\varphi_P + \varphi_W}{2} \tag{8}$$

$$\left(\Gamma A \frac{\partial \varphi}{\partial x}\right)_e - \left(\Gamma A \frac{\partial \varphi}{\partial x}\right)_w = \Gamma_e A_e \frac{\varphi_E - \varphi_P}{\Delta x_e} - \Gamma_w A_w \frac{\varphi_P - \varphi_W}{\Delta x_w} \tag{9}$$

then the conservation equation can be rewritten as:

$$\begin{aligned} &\left[\left(\frac{\Gamma_e A_e}{\Delta x_e} + \frac{\Gamma_w A_w}{\Delta x_w}\right) + \left(\frac{\Gamma_n A_n}{\Delta y_n} + \frac{\Gamma_s A_s}{\Delta y_s}\right) + \left(\frac{\Gamma_o A_o}{\Delta z_o} + \frac{\Gamma_i A_i}{\Delta z_i}\right) - S_P \Delta V\right] \varphi_P \\ &= \left(\frac{\Gamma_e A_e}{\Delta x_e} + \frac{(\rho u)_e A_e}{2}\right) \varphi_E + \left(\frac{\Gamma_w A_w}{\Delta x_w} + \frac{(\rho u)_w A_w}{2}\right) \varphi_W + \left(\frac{\Gamma_n A_n}{\Delta y_n} + \frac{(\rho u)_n A_n}{2}\right) \varphi_N \\ &+ \left(\frac{\Gamma_s A_s}{\Delta y_s} + \frac{(\rho u)_s A_s}{2}\right) \varphi_S + \left(\frac{\Gamma_o A_o}{\Delta z_o} + \frac{(\rho u)_o A_o}{2}\right) \varphi_o + \left(\frac{\Gamma_i A_i}{\Delta z_i} + \frac{(\rho u)_i A_i}{2}\right) \varphi_I + S_c \Delta V \end{aligned} \tag{10}$$

Replace the coefficient of each φ with a, and the discretization equation at each control point P can be expressed with a linear equation:

$$a_P\varphi_P = a_E\varphi_E + a_W\varphi_W + a_N\varphi_N + a_S\varphi_S + a_O\varphi_o + a_I\varphi_I + S_c\Delta V \tag{11}$$

Adjust the equations in the whole field using boundary equations, and the equations can be solved as a system of linear equations. It should be noted that Central Differencing Scheme is used in Eq (9), which owns better precision yet requires a small step length and small difference between flow in different directions. There are also upwind differencing schemes, hybrid differencing schemes, power-law differencing schemes and quadratic upstream interpolation for convective kinetics (QUICK), which mainly vary in different considerations of convection and diffusion.

As FVM is based on the conservation within a volume, its accuracy is less dependent on the volume size than FDM, but the solutions near the boundaries are not well-defined. Besides, the linear model used in discretization reduces its effectiveness in nonlinear dynamics. Given its drawbacks, FVM is still widely applied in commercial CFD analysis systems.

2.1.3. FEM. As a mature method that has been fully developed, FEM has been applied in current business software. For a governing equation u(x)=0, it can be expressed in integral form according to variation calculus:

$$\int_{\Omega} u(\boldsymbol{x})\delta u d\Omega = 0 \tag{12}$$

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where Ω represents a field and u is the function of space variable $\boldsymbol{x}$ defined in Ω. It can also transform into a weak integral form via integration by parts, which is more convenient for the following analysis. In FEM, the field is divided into finite element areas, often line segments in 1D, triangles in 2D and tetrahedrons in 3D cases. u is expressed as the sum of approximation functions $u^{(e)}$, which can be approximated by the linear combination of a series of primary functions ${\Phi_i}^{(e)}$:

$$u = \sum_e u^{(e)} \tag{13}$$

$$u^{(e)} = \sum_i u_i^{(e)} {\Phi_i}^{(e)} \tag{14}$$

where e stands for each element, and i walks through all the nodes of the element. Approximate the primary function ${\Phi_i}^{(e)}$ with linear functions, so ${\Phi_i}^{(e)}$ satisfies:

$${\Phi_i}^{(e)}\left({\boldsymbol{x}_j}^{(e)}\right) = \delta_{ij} \tag{15}$$

$${\Phi_i}^{(e)}\left({\boldsymbol{x}_j}^{(e)}\right) = a_i + b_i {x_j}^{(e)} + c_i {y_j}^{(e)} + d_i {z_j}^{(e)} \tag{16}$$

Thus, for each element, ${\Phi_i}^{(e)}$ can be solved as the coefficients of each $u^{(e)}$ in the weak integral FEM equations. Thus, the equations turn into a system of linear equations that can be solved by Gauss-Jordan elimination or nonlinear equations that can turn into linear ones via Newton-Raphson or other linearization algorithms.

2.2. Time discretization

2.2.1. Time domain marching method. One way to tackle unsteady flow problems is to treat the flow as steady flow and calculate the target function u at the beginning moment. Then, the value of u at any moment along the timeline can be given using the initial value and the values calculated in the former moments. Generally, the time discretization can be expressed as:

$$\frac{d\varphi^n}{dt} = \frac{(1+\alpha)\left(\varphi^{n+1}-\varphi^n\right)+\alpha\left(\varphi^n-\varphi^{n-1}\right)}{\Delta t} \tag{17}$$

where φ^n is the value at the nth time step, and α equals different constants in different discretization schemes, making the accuracy and stability vary. However, the inverse matrix with a high order is needed when solving the governing equations using such discretization, which requires mass calculation resources. Thus, dual time stepping method was proposed to improve calculation efficiency:

$$\left(\frac{d\varphi^n}{dt}\right)_{dual} = \frac{d\varphi^n}{d\tau} + \frac{(1+\alpha)\left(\varphi^{n+1}-\varphi^n\right)+\alpha\left(\varphi^n-\varphi^{n-1}\right)}{\Delta t} \tag{18}$$

where τ is pseudo time introduced to increase the internal iterations and improve accuracy. Such time domain marching method applies to any unsteady flow and is easy to understand. However, the method with higher than 3rd order can lead to divergence and extremely low efficiency because of the increasing time steps.

2.2.2. Frequency domain harmonic method. In many engineering conditions, the flow is periodical, offering convenience for developing and applying the frequency domain harmonic method. In a linear model, any variable φ can be expressed as the sum of time-averaged term $\overline{\varphi}$ and pulsation term φ':

$$\varphi = \overline{\varphi} + \varphi' \tag{19}$$

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In steady flow circumstances, the time-averaged terms can be solved, transforming the problem into solving the pulsation terms. In periodical flows, φ' is supposed to have the form:

$$\varphi'(\boldsymbol{x}, t) = \widetilde{\varphi}'(\boldsymbol{x})e^{jwt}$$

which is much simpler to tackle with. For models with nonlinearity, unsteady stress terms are introduced, which will not be specifically discussed in the article.

2.2.3. Time domain collocation method. The time domain collocation method is a general type of time discretization scheme projecting a variable that varies with time to a series of orthogonal subspaces of time and solving the steady flow problem in each subspace. One of the most mature methods is time spectral (TS) proposed by Gopinath [5], which gives the form of subspaces with Fourier transformation. In this approach, the variables can be solved in each time domain, thus at each periodically steady state. The method improved by one order of magnitude in calculation efficiency without reducing calculating accuracy. Apart from TS, other types of time domain collocation methods exist using different subspaces. Generally, the method applies to periodic flow with low frequency.

2.3. Summary

Direct numerical methods mainly simulate unsteady flow by solving the governing equations numerically and displaying the value of variables at every moment. Such methods have been widely applied in various areas, including studying wind flow around buildings, jet tanks, etc. Mature as they have been, spatial and time analysis optimizations in traditional numerical methods are still needed to improve calculating efficiency and reduce the CPU required, which points out the main future direction. Recently, Carlberg et al. proposed a two-stage strategy to reduce the data storage of CFD using machine learning to achieve dimensionality reduction and dynamic study [6]. Duffin et al. presented a statistical finite element method via the Bayesian approach to tackle nonlinear internal waves [7]. Uriarte and co-workers developed a dynamic deep-learning solver for linear PDEs using FEM [8].

3. Model for turbulence

Showing extreme irregularity and randomness, the turbulence model is one of the important factors affecting the accuracy of CFD calculation, which is necessary to carry out continuous and in-depth research [9]. The calculation DNS required in engineering makes the method only realizable for simple turbulence with low Reynolds numbers, which is far from practical use. To address the problem, many low- resolution approaches, including Reynolds Averaged N-S(RANS), Large Eddy Simulation (LES), and Detached Eddy Simulation (DES), arose in succession.

3.1. Reynolds averaged N-S (RANS)

Instead of calculating the pulsation term in all scales, RANS only considers the average information at all moments. From Eq. (19), the general variable φ is discomposed into the sum of $\overline{\varphi}$ and φ', with φ' in the following form:

$$\overline{\varphi} = \frac{1}{\Delta t}\int_{t}^{t+\Delta t} \varphi(t)dt$$

Replace each variable in the N-S equations with the form above; the general governing equations of turbulence can be written as:

$$\begin{cases} \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho \overline{u}_i) = 0 \\ \frac{\partial}{\partial t}(\rho \overline{u}_i) + \frac{\partial}{\partial x_j}\left(\rho \overline{u}_i \overline{u}_j\right) = \rho \overline{f}_i - \frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial \overline{u}_i}{\partial x_j} - \rho \overline{\mu_i{}' \mu_j{}'}\right) \\ \frac{\partial(\rho \overline{\varphi})}{\partial t} + \frac{\partial\left(\rho \overline{\varphi} \overline{u}_j\right)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\Gamma_\varphi \frac{\partial \overline{\varphi}}{\partial x_j} - \rho \overline{\varphi'^{\mu_j}}\right) + S_\varphi \end{cases} \tag{20}$$

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where the pulsing of density is omitted and Reynolds stress $\tau_{ij} = -\rho\overline{\mu_i'\mu_j'}$ is introduced, making the equation set unclosed.

To deal with τ_{ij}, Turbulent Viscosity Model is developed, with Boussinesq first proposing the turbulent viscosity assumption in 1887:

$$-\rho\overline{\mu_i'\mu_j'} = \mu_t\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}\left(\rho k+\mu\frac{\partial u_i}{\partial x_i}\right)\delta_{ij} \tag{21}$$

where the scalar function μ_t is the turbulent viscosity and k is the turbulent kinetic energy. Since the 1920s, more and more models have been developed to establish the relationship between μ_t and the flow. In 1924, Prandtl proposed the mixing length model, supposing that μ_t is proportional to $\nabla u_i \cdot l_m^2$, where l_m is mixing length representing the distance fluid micelles have covered before dissipation and is an experience value. Based on the mixing length theory, many classic models were proposed, including the SA model by Sparlart in 1992 [10], $k-\varepsilon$ model by Launder and Spalding in 1974 [11], as well as $k-\varepsilon$ model published by Wilcox in 2008 after a three-decade improvement in its original form proposed in the 1970s [12].

3.1.1. The standard $k-\varepsilon$ model (STD). STD gives the relationship of turbulent kinetic energy k, turbulent dissipation rate ε and the flow variables to describe μ_t:

$$k = \frac{\overline{u'^2+v'^2+w'^2}}{2} \tag{22}$$

$$\varepsilon = \frac{\mu}{\rho}\overline{\left(\frac{\partial u_i'}{\partial x_k}\right)\left(\frac{\partial u_i'}{\partial x_k}\right)} \tag{23}$$

$$\mu_t = \rho C_\mu \frac{k}{\varepsilon^2} \tag{24}$$

where C_μ is an experience value. As two extra variables k and ε are introduced, their transport equations are used to make the equations closed:

$$\frac{\partial(\rho k)}{\partial t}+\frac{\partial(\rho k u_i)}{\partial x_i} = \frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]+G_k+G_b-\rho\varepsilon-Y_M+S_k \tag{25}$$

$$\frac{\partial(\rho\varepsilon)}{\partial t}+\frac{\partial(\rho\varepsilon u_i)}{\partial x_i} = \frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right]+C_{1\varepsilon}\frac{\varepsilon}{k}\left(G_k+C_\mu G_b\right)-C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}+S_\varepsilon \tag{26}$$

where $C_{1\varepsilon}$, $C_{2\varepsilon}$ and C_μ are experience values, σ_k and σ_ε are the corresponding Prandtl coefficients, G_k does velocity gradient while causing an extra term G_b is caused by buoyancy, and Y_M is a result of pulsating expansion [13]. Because of the experience values, the STD $k-\varepsilon$ model mainly addresses complex and fully developed turbulence, where the Reynolds number is relatively large. The model has its restriction regarding laminar flow, where viscosity between molecules has more effect than Reynolds stress, as well as high-rotational or curved flow.

3.1.2. The renormalization group $k-\varepsilon$ model (RNG). On account of the STD model, Yakhot and Orzag developed RNG in 1986 [14]:

$$\frac{\partial(\rho k)}{\partial t}+\frac{\partial(\rho k u_i)}{\partial x_i} = \frac{\partial}{\partial x_j}\left[1.39(\mu+\mu_t)\frac{\partial k}{\partial x_j}\right]+G_k-\rho\varepsilon \tag{27}$$

$$\frac{\partial(\rho\varepsilon)}{\partial t}+\frac{\partial(\rho\varepsilon u_i)}{\partial x_i} = \frac{\partial}{\partial x_j}\left[1.39(\mu+\mu_t)\frac{\partial \varepsilon}{\partial x_j}\right]+C_{1\varepsilon}{}^*\frac{\varepsilon}{k}G_k-C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} \tag{28}$$

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with ${C_{1\varepsilon}}^*$, η and E_{ij} expressed as:

$$ {C_{1\varepsilon}}^* = C_{1\varepsilon} - \frac{\eta\left(1-\frac{\eta}{4.377}\right)}{1+0.012\eta^3}, \eta = \sqrt{2}E_{ij}\frac{k}{\varepsilon}, E_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right) $$

where the effective turbulent viscosity $\mu_{eff} = \mu + \mu_t$ reflects a modification in turbulent viscosity considering flow rotation, and time mean strain rate E_{ij} takes a spatial variation of the extra terms into account [13]. Therefore, the RNG $k-\varepsilon$ model performs better in dealing with the curved flow. Apart from the STD and RNG $k-\varepsilon$ models, there are also other derivatives of the $k-\varepsilon$ model, including the realizable $k-\varepsilon$ model, and the paper will not go into details about them here.

3.1.3. The $k-\omega$ model. The $k-\omega$ model is another approach to describe μ_t. The experience values in $k-\varepsilon$ model greatly depend on the damping function at the viscous sublayer, which may be inaccurate in flows with a high adverse pressure gradient. The $k-\omega$ model is free of this problem with the introduction of specific dissipation rate ω, and the model equations are as follows:

$$ \frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho k u_j)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\mu + \sigma^*\frac{\rho k}{\omega}\right)\frac{\partial k}{\partial x_j}\right] + \tau_{ij}\frac{\partial u_i}{\partial x_j} - \beta^*\rho k\omega \tag{29} $$

$$ \frac{\partial(\rho\omega)}{\partial t} + \frac{\partial(\rho\omega u_j)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\mu + \sigma\frac{\rho k}{\omega}\right)\frac{\partial \omega}{\partial x_j}\right] + \alpha\frac{\omega}{k}\tau_{ij}\frac{\partial u_i}{\partial x_j} - \beta\rho\omega^2 + \sigma_d\frac{\rho}{\omega}\frac{\partial k}{\partial x_j}\frac{\partial \omega}{\partial x_j} \tag{30} $$

where ω is the specific dissipation rate differing from the dissipation rate ε, and α, σ^* and β^* are closure coefficients. The $k-\omega$ model significantly enhanced the prediction of many categories of free-shear-flow, including mixing layer and plane jet, and reduced the influence caused by varied freestream boundary conditions. Furthermore, in 1992, the SST model was proposed by Menter, introducing a cross-diffusion term to the ω equation above, which achieved the transition and transformation between $k-\varepsilon$ and $k-\omega$ model. At present, SST is more widely used in commercial CFD engineering.

3.2. Large eddy simulation (LES)

Initially proposed in the 1970s, LES distinguishes the fluid on a large scale from that on a small scale, establishing a pulsation model to simulate the latter. For a general variable φ, LES defines its filtered form:

$$ \overline{\varphi}(x) = \int_D \varphi(x')G(x,x')dx' $$

where G is the filtration function, and D represents the definition area of the fluid. While RANS establishes the governing equation of the time-averaged term, LES sets governing equations of the filtered term $\overline{\varphi}$:

$$ \begin{cases} \frac{\partial\rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho\overline{u_i}) = 0 \\ \frac{\partial}{\partial t}(\rho\overline{u_i}) + \frac{\partial}{\partial x_j}(\rho\overline{u_i}\overline{u_j}) = \frac{\partial}{\partial x_j}\left(\mu\frac{\partial\overline{u_i}}{\partial x_j}\right) - \frac{\partial\overline{p}}{\partial x_i} - \frac{\partial\tau_{ij}}{\partial x_i} \\ \tau_{ij} = \rho\overline{u_i u_j} - \rho\overline{u_i}\overline{u_j} \end{cases} \tag{31} $$

where the extra term τ_{ij} is called sub-grid stress describing turbulence behaviors whose scale is less than the filter scale [13]. To solve τ_{ij}, eddy model is mostly used:

$$ \tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} = -2\mu_t\overline{S_{ij}} \tag{32} $$

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$$\overline{S_{ij}} = \frac{1}{2}\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right) \tag{33}$$

where μ_t represents subgrid turbulent viscosity and $\overline{S_{ij}}$ is the stress ratio tensor under the filtered scale [13].

For the solution of μ_t, Smagorinsky proposed the most initial model [15]:

$$\mu_t = \rho\sqrt{2\overline{S_{ij}S_{ij}}}\cdot l_s^2 \tag{34}$$

$$l_s = \min\left(0.42d, C_s V^{\frac{1}{3}}\right) \tag{35}$$

where l_s is the mixing length of the subgrid and d stands for the distance between fluid micelle and wall, and V is the control volume. C_s is a constant whose value was given as 0.23 and corrected as 0.1, which shows better simulation performance. Additionally, there's a subgrid model based on the renormalization group theory giving $\mu_{eff} = \mu + \mu_t$ with the form:

$$\mu_{eff} = \mu\left[1 + H\left(\frac{\mu_s^2\mu_{eff}}{\mu^3} - 100\right)\right]^{\frac{1}{3}} \tag{36}$$

$$\mu_s = 0.246V^{\frac{2}{3}}\sqrt{2\overline{S_{ij}S_{ij}}} \tag{37}$$

where H is the Heaviside function, and V is the control volume.

3.3. Detached eddy simulation (DES)

Initially proposed in 1997, DES combines RANS and LES to make a compromise between calculation efficiency and accuracy in turbulence. Through analyzing turbulent flows in a filtered scale, LES is able to give more accurate simulations. However, more compact meshes are also required in this method, adding to more calculations and low efficiency, especially at the boundary layer near the wall. Therefore, RANS is used near the wall, while on a larger scale, LES is applied. According to different models used in RANS and LES, there're several DES model equations, and one of the most widely applied ones is based on the SST model in RANS, proposed by Strelets [16], with the governing equations expressed as:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho k u_j)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + \tau_{ij}\frac{\partial u_i}{\partial x_j} - \beta^*\rho k\omega\cdot F_{DES} \tag{38}$$

$$\frac{\partial(\rho\omega)}{\partial t} + \frac{\partial(\rho\omega u_j)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\omega}\right)\frac{\partial \omega}{\partial x_j}\right] + \alpha\frac{\omega}{k}\tau_{ij}\frac{\partial u_i}{\partial x_j} - \beta\rho\omega^2 + 2(1-F_1)\sigma_{\omega_2}\frac{\rho^2}{\omega}\frac{\partial k}{\partial x_j}\frac{\partial \omega}{\partial x_j} \tag{39}$$

where σ_{ω_2} is constant, F_1 is the Menter's blending function designed to be one in the near-wall region and zero away from the surface [17]. And the switching function F_{DES} is introduced to control the equations according to the distance between the control volume and the wall, with the form:

$$F_{DES} = \max\left\{\frac{l_{k-\omega}}{C_{DES}\Delta}, 1\right\}$$

where $l_{k-\omega} = \frac{\sqrt{k}}{\beta^*\omega}$ is the length scale of the RANS model, Δ is the maximum grid distance and C_{DES} is an experience value.

Although DES performs well in complicated turbulence, it appears to depend on meshes due to the obscure border between RANS and LES area. A delay factor was introduced to protect the boundary

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layer, and thus DDES was proposed to optimize DES, which made some modifications in the switching function. Still, take SST-DDES as an example:

$$F_{DDES} = \max\left\{(1 - F_{SST})\frac{l_{k-\omega}}{C_{DES}\Delta}, 1\right\}$$
$$F_{SST} = F_1 \; or \; F_2$$

where F_2 is similar to F_1, a boundary-identification function defined in the SST model.

3.4. Summary

RANS, LES and DES are operated by filtering certain terms in governing equations and expressing the filtered articles with modeled terms and are widely used in turbulence simulation. Among them, RANS replaces the details on the time scale with the Reynolds stress term. In comparison, LES ignores the details on the space scale using the subgrid term. Therefore, the two methods share a similar form of governing equations, with RANS being more efficient yet less accurate and LES providing more comprehensive information on fluid fields with denser meshes, leading to more calculations. Therefore, various methods of mixing RANS/LES were proposed [18], with DES being the earliest and most widely used one and DDES optimizing DES in terms of influence caused by local turbulence. At present, this series of methods have been widely applied in engineering. Using SST, Liu et al. developed a CFD solver for multidimensional compressible flow [19]. Wang et al. provided references for simulations of high rotational flows by applying a series of models, including URANS, SST, DES, etc. [20]. Zamiri et al. compared LES, SAS and DES when simulating the film-cooling process and predicted turbulence and film-cooling effectiveness in a fan-shaped hole [21].

4. Reduced order model (ROM)

An extreme drawback of traditional numerical methods of CFD lies in the tremendous, massive calculation required, taking up too much calculation resources and computing time. Besides, people cannot pinpoint the key features of a fluid field by merely solving differential equations. Therefore, several types of ROM have been proposed since the 1990s to describe major characteristics of the fluid field with fewer degrees of freedom and thus less calculation, and till now, the model has been considered another breakthrough in aeroelasticity.

4.1. ROM based on system identification

This type of ROM establishes the reflection between the input and output data using mathematical approaches. Some representative theories include the Volterra series, linear autoregressive moving average (ARMA), radio basis function (RBF) neural network, etc. Due to the limited space, only the first one will be extended in detail.

The continuous Volterra series can be expressed as:

$$\begin{aligned} y(t) = H_0 + \int_0^t H_1(t-\tau_1)u(\tau_1)d\tau_1 + \ldots \int_0^t \int_0^t H_2(t-\tau_1, t-\tau_2)u(\tau_1)u(\tau_2)d\tau_1 d\tau_2 \\ + \int_0^t \ldots \int_0^t H_k(t-\tau_1, \ldots, t-\tau_k) \prod_{i=1}^k [u(\tau_i)d\tau_i] \end{aligned} \quad (40)$$

while the discrete form reads:

$$\begin{aligned} y(n) = H_0 + \sum_{m_1=0}^n H_1(n-m_1)u(m_1) + \sum_{m_1=0}^n \sum_{m_2=0}^n H_2(n-m_1, n-m_2)u(m_1)u(m_2) + \ldots \\ + \sum_{m_1=0}^n \ldots \sum_{m_k=0}^n H_k(n-m_1, \ldots, n-m_k) \prod_{i=1}^k u(m_i) \end{aligned} \quad (41)$$

where $u(n)$ represents the input while $y(n)$ represents the response, $n = 0,1,2, \ldots$ is the discrete-time variables, and H_k is the k-order Volterra operator. In practical use, only a 1- or 2-order Volterra operator is sufficient to precisely describe the characteristics; thus, it's not hard to obtain the Volterra kernel $H_k(n)$.

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4.2. ROM based on feature extraction

The core theory of this kind of ROM is to seek a group of low-dimensional subspaces on which flow behaviors in high-dimensional space can be reflected to reduce the complexity of the fluid field and describe and predict the variables in the field. To construct the subspaces, a great amount of data has to be collected, and the typical methods include the Koopman operator, Proper Orthogonal Decomposition (POD) and Dynamic Model Decomposition (DMD), with the latter two introduced in detail as follows.

4.2.1. Proper orthogonal decomposition (POD). Dating back to the K-L transformation proposed in the 1940s, POD extracts a series of snapshots as samples and seeks orthogonal subspaces with the lower order to analyze the key characteristics in the fluid field. Consider a series of snapshots in N moments $\boldsymbol{u}(\boldsymbol{x}, t_i)$, discomposing each of them into the sum of time-averaged term $\boldsymbol{u}_0(\boldsymbol{x})$ and pulsation term $\boldsymbol{u}'(\boldsymbol{x}, t_i)$, while $\boldsymbol{u}'(\boldsymbol{x}, t_i)$ can be expressed with fewer primary functions $\boldsymbol{\phi}_j(\boldsymbol{x})$:

$$\boldsymbol{u}(\boldsymbol{x}, t_i) = \boldsymbol{u}_0(\boldsymbol{x}) + \boldsymbol{u}'(\boldsymbol{x}, t_i), i = 1,2, ..., N \tag{42}$$

$$\boldsymbol{u}'(\boldsymbol{x}, t_i) = \sum_{j=1}^{M} a_j(t_i)\, \boldsymbol{\phi}_j(\boldsymbol{x}), 0 < M < N \tag{43}$$

where $a_j(t_i)$ is the jth modal coefficient of each time step t_i. Define the snapshot matrix $\boldsymbol{P}$:

$$\boldsymbol{P} = \left[\boldsymbol{u}'(\boldsymbol{x}, t_1), \boldsymbol{u}'(\boldsymbol{x}, t_2), ..., \boldsymbol{u}'(\boldsymbol{x}, t_N) \right]$$

And the primary matrix of the orthogonal subspace:

$$\boldsymbol{\Phi} = [\boldsymbol{\phi}_1(\boldsymbol{x}), \boldsymbol{\phi}_2(\boldsymbol{x}), ..., \boldsymbol{\phi}_M(\boldsymbol{x})]$$

As the error between the snapshots and the orthogonal subspace should be minimized, written as:

$$min \sum_{i=1}^{N} \left\| \boldsymbol{u}'(\boldsymbol{x}, t_i) - \boldsymbol{\Phi}\boldsymbol{\Phi}^{\boldsymbol{H}} \boldsymbol{u}'(\boldsymbol{x}, t_i) \right\| \tag{44}$$

So $\boldsymbol{\Phi}$ should be maximized. Through standardizing:

$$\boldsymbol{J}(\boldsymbol{\Phi}) = \sum_{i=1}^{N} \left(\boldsymbol{u}'(\boldsymbol{x}, t_i), \boldsymbol{\Phi} \right)^2 - \lambda(|| \boldsymbol{\Phi}|| - \boldsymbol{1})$$

Set $\frac{d}{d\boldsymbol{\Phi}} \boldsymbol{J}(\boldsymbol{\Phi}) = 0$, the original problem turns into:

$$\left(\boldsymbol{P}\boldsymbol{P}^H - \lambda I \right) \boldsymbol{\Phi} = \boldsymbol{0} \tag{45}$$

and can be further simplified to an eigenvalue problem:

$$\begin{cases} \boldsymbol{P}^H \boldsymbol{P}\boldsymbol{A} = \boldsymbol{\Lambda}\boldsymbol{A} \\ \boldsymbol{\Phi} = \boldsymbol{\Lambda}^{-\frac{\boldsymbol{1}}{\boldsymbol{2}}} \boldsymbol{P}\boldsymbol{A} \end{cases} \tag{46}$$

where

$$\boldsymbol{A} = \left[\boldsymbol{A}^{[1]}, \boldsymbol{A}^{[2]}, ..., \boldsymbol{A}^{[M]} \right], \ \boldsymbol{A}^{[j]} = \begin{bmatrix} a_j(t_1) \\ a_j(t_2) \\ a_j(3) \\ ... \\ a_j(t_N) \end{bmatrix}$$

and $\boldsymbol{\Lambda}$ is the eigenvalue matrix. According to the eigenvalues λ_j, major models can be extracted to analyze the general fluid field at a low cost.

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4.2.2. Dynamic model decomposition (DMD). DMD is another approach to reducing the order of the fluid field, which was first proposed by Schmid in 2008 [22]. Based on a linear dynamic process, DMD establishes two snapshot series:

$$\boldsymbol{X} = [\boldsymbol{x_1}, \boldsymbol{x_2}, ..., \boldsymbol{x_{N-1}}]$$
$$\boldsymbol{Y} = [\boldsymbol{x_2}, \boldsymbol{x_3}, ..., \boldsymbol{x_N}]$$

with the relationship

$$\boldsymbol{Y} = [\boldsymbol{Ax_1}, \boldsymbol{Ax_2}, ..., \boldsymbol{Ax_{N-1}}] = \boldsymbol{AX} \tag{47}$$

One way to approximate $\boldsymbol{A}$ is through a companion matrix. Suppose the following relationships:

$$\boldsymbol{x_N} = c_1\boldsymbol{x_1} + c_2\boldsymbol{x_2} + ... + c_{N-1}\boldsymbol{x_{N-1}} \tag{48}$$

Thus, there is:

$$\boldsymbol{AX} = \boldsymbol{XS} \tag{49}$$

where $\boldsymbol{S}$ is the companion matrix of $\boldsymbol{A}$. $\boldsymbol{S}$ can be constructed by minimizing the difference between $\boldsymbol{x_N}$ and $\sum_{\boldsymbol{i=1}}^{\boldsymbol{N-1}} c_i\boldsymbol{x_i}$, so the eigenvalues of $\boldsymbol{A}$ can be given. Besides, another way to get the eigenvalues of $\boldsymbol{A}$ is by replacing $\boldsymbol{A}$ with its similar matrix with the lower order. Compared with POD, DMD simplifies linearity while straightforwardly giving the eigenvalues of the fluid field modal and displaying the time evolution.

4.3. Summary

Thanks to ROM, more concise and efficient approaches are developed to provide accurate information on the key characteristics of fluid fields, which is helpful for an in-depth understanding of unsteady flow and analysis for complex fluid fields with high orders. In recent years, Li et al. presented a more efficient CFD-based ROM model, improving the robustness of ROM to aeroelastic systems by applying Genetic Algorithms (GA) [23]. Chen et al. proposed a new ROM model, doing interpolation in tangent space to the Grassmann manifold to get the POD matrix and using the least squares support vector machine (LS-SVM) to associate the excitations and POD to establish the ROM, which has great prospect in predicting hypersonic unsteady aerodynamic flow [24]. Casas et al. combined ROM with Data Assimilation and machine learning and constructed a Reduced Order Deep Data Assimilation (RODDA) model containing a neural network trained by data provided by CFD and can predict fluid fields with higher accuracy [25]. Pant et al. developed a nonlinear projection framework for ROM based on deep learning, which can predict the future time step without supervision and thus save plenty of calculations [26]. Aversano et al. applied the technic to flameless combustion, presenting a ROM digital twin to predict the state variables of chemical reactions based on data compression via POD [27].

5. Conclusions

The paper reviewed the main computational methods developed since the emergence of CFD. First, the governing equations were displayed, including the most classic N-S and other derived equations like Euler and full potential. Other governing equations are also based on different fluid dynamic conditions, but their core articles are all fluid field variables' spatial and time derivatives. Then the methods based on three different theories are listed. Actually, with the evolution of CFD in the last 50 years, not all the computational methods are covered in this paper, for instance, finite analytic method (FAM), grid generation and lattice Boltzmann model (LBM), but the approaches displayed have been relatively representative. The key idea for DNS is to solve the ODEs or PDEs using numerical methods, which were divided into spatial and time discretization schemes for discussion. However, as too much calculation is required in DNS, new methods needed to be applied to reduce computation complexity with less reduction in accuracy, which facilitated a series of methods represented by RANS, LES and DES. Furthermore, ROM represents another approach to address CFD problems,

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reducing calculation while giving a better view of the intrinsic qualities of fluid fields. ROM can be further classified into system identification and feature extraction. There is still great room for improvement in ROM, especially its combination with machine learning or other AI algorithms. With the development of ROM, aerodynamic modeling of unsteady flow can be further optimized, which is vital for the flow control design.

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