

METHODS INVOLVED IN SOLVING PROBLEMS OF FLUID MECHANICS USING COMPUTATIONAL FLUID DYNAMICS- A STUDY

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ABSTRACT

This research paper offers an overview of the techniques used to solve problems in fluid mechanics using computational fluid dynamics (CFD) on computers and describes in detail those most often used in practice. Included are advanced methods in computational fluid dynamics, like direct and large-eddy simulation of turbulence, Probability density function (PDF) methods and vortex methods. It also contains a section dealing with grid quality and an extended description of discretization methods like finite element method (FEM), finite volume method (FVM), finite difference method (FDM) and boundary element method. This paper shows common roots and basic principles for many different methods.

Keywords: *Fluid Dynamics, Navier–Stokes equations, Hydrodynamics, Boundary layer flow, Computational Fluid Dynamics.*

INTRODUCTION

Computational fluid dynamics (CFD) is a branch of fluid mechanics that uses numerical methods and algorithms to solve and analyze problems that involve fluid flows. Computers are used to perform the calculations required to simulate the interaction of liquids and gases with surfaces defined by boundary conditions. With high-speed supercomputers, better solutions can be achieved. Ongoing research, however, yields software that improves the accuracy and speed of complex simulation scenarios such as transonic or turbulent flows. Initial validation of such software is performed using a wind tunnel with the final validation coming in flight tests.

The fundamental basis of almost all CFD problems is the Navier–Stokes equations, which defines any single-phase fluid flow. These equations can be simplified by removing terms describing viscosity to yield the Euler equations. Further simplification, by removing terms describing vorticity yields the full potential equations. Finally, these equations can be linearized to yield the linearized potential equations.

The Navier–Stokes equations were the ultimate target of developers. Two-dimensional codes, such as NASA Ames' ARC2D code first emerged. A number of three-dimensional codes were developed (ARC3D, OVERFLOW, CFL3D are three successful NASA contributions), leading to numerous commercial packages.

METHODOLOGY

In all of these approaches the same basic procedure is followed.

- *During preprocessing*
 - The geometry (physical bounds) of the problem is defined.
 - The volume occupied by the fluid is divided into discrete cells (the mesh). The mesh may be uniform or non uniform.
 - The physical modeling is defined – for example, the equations of motions + enthalpy + radiation + species conservation
 - Boundary conditions are defined. This involves specifying the fluid behavior and properties at the boundaries of the problem. For transient problems, the initial conditions are also defined.
- The simulation is started and the equations are solved iteratively as a steady-state or transient.
- Finally a postprocessor is used for the analysis and visualization of the resulting solution.

Discretization methods

The stability of the chosen discretization is generally established numerically rather than analytically as with simple linear problems. Special care must also be taken to ensure that the discretization handles discontinuous solutions gracefully. The Euler equations and Navier–Stokes equations both admit shocks, and contact surfaces. Some of the discretization methods being used are:

Finite volume method

The finite volume method (FVM) is a common approach used in CFD codes. The governing equations are solved over discrete control volumes. Finite volume methods recast the governing partial differential equations (typically the Navier-Stokes equations) in a conservative form, and then discretize the new equation. This guarantees the conservation of fluxes through a particular control volume. Though the overall solution will be conservative in nature, there is no guarantee that it is the actual solution. The finite volume equation yields governing equations in the form,

$$\frac{\partial}{\partial t} \iiint Q dV + \iint F d\mathbf{A} = 0,$$

where Q is the vector of conserved variables, F is the vector of fluxes (see Euler equations or Navier–Stokes equations), V is the volume of the control volume element, and A is the surface area of the control volume element.

Finite element method

The finite element method (FEM) is used in structural analysis of solids, but is also applicable to fluids. However, the FEM formulation requires special care to ensure a conservative solution. The FEM formulation has been adapted for use with fluid dynamics governing equations. Although FEM must be carefully formulated to be conservative, it is much more stable than the finite volume approach^[4] However, FEM can require more memory than FVM.^[5]

In this method, a weighted residual equation is formed:

$$R_i = \iiint W_i Q dV^e$$

where R_i is the equation residual at an element vertex i , Q is the conservation equation expressed on an element basis, W_i is the weight factor, and V^e is the volume of the element.

Finite difference method

The finite difference method (FDM) has historical importance and is simple to program. It is currently only used in few specialized codes. Modern finite difference codes make use of an embedded boundary for handling complex geometries, making these codes highly efficient and accurate. Other ways to handle geometries include use of overlapping grids, where the solution is interpolated across each grid.

$$\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} = 0$$

where Q is the vector of conserved variables, and F , G , and H are the fluxes in the x , y , and z directions respectively.

Boundary element method

In the boundary element method, the boundary occupied by the fluid is divided into a surface mesh.

High-resolution discretization schemes

High-resolution schemes are used where shocks or discontinuities are present. Capturing sharp changes in the solution requires the use of second or higher-order numerical schemes that do not introduce spurious oscillations. This usually necessitates the application of flux limiters to ensure that the solution is total variation diminishing.

Turbulence models

In studying turbulent flows, the objective is to obtain a theory or a model that can yield quantities of interest, such as velocities. For turbulent flow, the range of length scales and complexity of phenomena make most approaches impossible. The primary approach in this case is to create numerical models to calculate the properties of interest. A selection of some commonly-used computational models for turbulent flows is presented in this section.

The chief difficulty in modeling turbulent flows comes from the wide range of length and time scales associated with turbulent flow. As a result, turbulence models can be classified based on the range of these length and time scales that are modeled and the range of length and time scales that are resolved. The more turbulent scales that are resolved, the finer the resolution of the simulation, and therefore the higher the computational cost. If a majority or all of the turbulent scales are modeled, the computational cost is very low, but the tradeoff comes in the form of decreased accuracy.

In addition to the wide range of length and time scales and the associated computational cost, the governing equations of fluid dynamics contain a non-linear convection term and a non-linear and non-local pressure gradient term. These nonlinear equations must be solved numerically with the appropriate boundary and initial conditions.

Direct numerical simulation

Direct numerical simulation (DNS) resolves the entire range of turbulent length scales. This marginalizes the effect of models, but is extremely expensive. The computational cost is proportional to Re^3 .^[6] DNS is intractable for flows with complex geometries or flow configurations.

Large eddy simulation

Large eddy simulation (LES) is a technique in which the smallest scales of the flow are removed through a filtering operation, and their effect modeled using sub grid scale models. This allows the largest and most important scales of the turbulence to be resolved, while greatly reducing the computational cost incurred by the smallest scales. This method requires greater computational resources than RANS methods, but is far cheaper than DNS.



Figure-1 Volume rendering of a non-premixed swirl flame as simulated by LES.

Detached eddy simulation

Detached eddy simulations (DES) is a modification of a RANS model in which the model switches to a subgrid scale formulation in regions fine enough for LES calculations. Regions near solid boundaries and where the turbulent length scale is less than the maximum grid dimension are assigned the RANS mode of solution. As the turbulent length scale exceeds the grid dimension, the regions are solved using the LES mode. Therefore the grid resolution for DES is not as demanding as pure LES, thereby considerably cutting down the cost of the computation. Though DES was initially formulated for the Spalart-Allmaras model (Spalart et al., 1997), it can be implemented with other RANS models (Strelets, 2001), by appropriately modifying the length scale which is explicitly or implicitly involved in the RANS model. So while Spalart-Allmaras model based DES acts as LES with a wall model, DES based on other models (like two equation models) behave as a hybrid RANS-LES model. Grid generation is more complicated than for a simple RANS or LES case due to the RANS-LES switch. DES is a non-zonal approach and provides a single smooth velocity field across the RANS and the LES regions of the solutions.

Reynolds-averaged Navier–Stokes equations

Reynolds-averaged Navier-Stokes (RANS) equations are the oldest approach to turbulence modeling. An ensemble version of the governing equations is solved, which introduces new apparent stresses known as Reynolds stresses. This adds a second order tensor of unknowns for which various models can provide different levels of closure. It is a common misconception that the RANS equations do not apply to flows with a time-varying mean flow because these equations are 'time-averaged'. In fact, statistically unsteady (or non-stationary) flows can equally be treated. This is sometimes referred to as URANS. There is nothing inherent in Reynolds averaging to preclude this, but the turbulence models used to close the equations are valid only as long as the time over which these changes in the mean occur is large compared to the time scales of the turbulent motion containing most of the energy.

RANS models can be divided into two broad approaches:

Boussinesq hypothesis

This method involves using an algebraic equation for the Reynolds stresses which include determining the turbulent viscosity, and depending on the level of sophistication of the model, solving transport equations for determining the turbulent kinetic energy and dissipation. Models include $k-\epsilon$ (Launder and Spalding),^[7] Mixing Length Model (Prandtl),^[8] and Zero Equation Model (Cebeci and Smith).^[8] The models available in this approach are often referred to by the number of transport equations associated with the method. For example, the Mixing Length model is a "Zero Equation" model because no transport equations are solved; the $k - \epsilon$ is a "Two Equation" model because two transport equations (one for k and one for ϵ) are solved.

Reynolds stress model (RSM)

This approach attempts to actually solve transport equations for the Reynolds stresses. This means introduction of several transport equations for all the Reynolds stresses and hence this approach is much more costly in CPU effort.

Coherent vortex simulation

The coherent vortex simulation approach decomposes the turbulent flow field into a coherent part, consisting of organized vortical motion, and the incoherent part, which is the random background flow.^[9] This decomposition is done using wavelet filtering. The approach has much in common with LES, since it uses decomposition and resolves only the filtered portion, but different in that it does not use a linear, low-pass filter. Instead, the filtering operation is based on wavelets, and the filter can be adapted as the flow field evolves. Farge and Schneider tested the CVS method with two flow configurations and showed that the coherent portion of the

flow exhibited the $-\frac{5}{3}$ energy spectrum exhibited by the total flow, and corresponded to coherent structures (vortex tubes), while the incoherent parts of the flow composed homogeneous background noise, which exhibited no organized structures. Goldstein and Oleg^[10] applied the CVS model to large eddy simulation, but did not assume that the wavelet filter completely eliminated all coherent motions from the sub filter scales. By employing both LES and CVS filtering, they showed that the SFS dissipation was dominated by the SFS flow field's coherent portion.

Probability density function (PDF) methods

Probability density function (PDF) methods for turbulence, first introduced by Lundgren,^[11] are based on tracking the one-point PDF of the velocity, $f_V(\mathbf{v}; \mathbf{x}, t)d\mathbf{v}$, which gives the probability of the velocity at point \mathbf{x} being between \mathbf{v} and $\mathbf{v} + d\mathbf{v}$. This approach is analogous to the kinetic theory of gases, in which the macroscopic properties of a gas are described by a large number of particles. PDF methods are unique in that they can be applied in the framework of a number of different turbulence models; the main differences occur in the form of the PDF transport equation. For example, in the context of large eddy simulation, the PDF becomes the filtered PDF.^[12] PDF methods can also be used to describe chemical reactions,^{[13][14]} and are particularly useful for simulating chemically reacting flows because the chemical source term is closed and does not require a model. The PDF is commonly tracked by using Lagrangian particle methods; when combined with large eddy simulation, this leads to a Langevin equation for subfilter particle evolution.

Vortex method

The vortex method is a grid-free technique for the simulation of turbulent flows. It uses vortices as the computational elements, mimicking the physical structures in turbulence. Vortex methods were developed as a grid-free methodology that would not be limited by the fundamental smoothing effects associated with grid-based methods. To be practical, however, vortex methods require means for rapidly computing velocities from the vortex elements – in other words they require the solution to a particular form of the N-body problem (in which the motion of N objects is tied to their mutual influences). A breakthrough came in the late 1980s with the development of the fast multipole method (FMM), an algorithm by V. Rokhlin (Yale) and L. Greengard (Courant Institute). This breakthrough paved the way to practical computation of the velocities from the vortex elements and is the basis of successful algorithms. They are especially well-suited to simulating filamentary motion, such as wisps of smoke, in real-time simulations such as video games, because of the fine detail achieved using minimal computation.^[15]

Software based on the vortex method offer a new means for solving tough fluid dynamics problems with minimal user intervention. All that is required is specification of problem geometry and setting of boundary and initial conditions. Among the significant advantages of this modern technology;

- *It is practically grid-free, thus eliminating numerous iterations associated with RANS and LES.*
- *All problems are treated identically. No modeling or calibration inputs are required.*
- *Time-series simulations, which are crucial for correct analysis of acoustics, are possible.*
- *The small scale and large scale are accurately simulated at the same time.*

Vorticity confinement method

The vorticity confinement (VC) method is an Eulerian technique used in the simulation of turbulent wakes. It uses a solitary-wave like approach to produce a stable solution with no numerical spreading. VC can capture the small scale features to within as few as 2 grid cells. Within these features, a nonlinear difference equation is solved as opposed to the finite difference equation. VC is similar to shock capturing methods, where conservation laws are satisfied, so that the essential integral quantities are accurately computed.

Two-phase flow

The modeling of two-phase flow is still under development. Different methods have been proposed. The Volume of fluid method has received a lot of attention lately, for problems that do not have dispersed particles, but the Level set method and front tracking are also valuable approaches. Most of these methods are either good in maintaining a sharp interface or at conserving mass. This is crucial since the evaluation of the density, viscosity and surface tension is based on the values averaged over the interface. Lagrangian multiphase models, which are used for dispersed media, are based on solving the Lagrangian equation of motion for the dispersed phase.

Solution algorithms

Discretization in space produces a system of ordinary differential equations for unsteady problems and algebraic equations for steady problems. Implicit or semi-implicit methods are generally used to integrate the ordinary differential equations, producing a system of (usually) nonlinear algebraic equations. Applying a Newton or Picard iteration produces a system of linear equations which is nonsymmetric in the presence of advection and indefinite in the presence of incompressibility. Such systems, particularly in 3D, are frequently too large for direct solvers, so iterative methods are used, either stationary methods such as successive overrelaxation

or Krylov subspace methods. Krylov methods such as GMRES, typically used with preconditioning, operate by minimizing the residual over successive subspaces generated by the preconditioned operator.

For indefinite systems, preconditioners such as incomplete LU factorization, additive Schwarz, and multigrid perform poorly or fail entirely, so the problem structure must be used for effective preconditioning.^[16] Methods commonly used in CFD are the SIMPLE and Uzawa algorithms which exhibit mesh-dependent convergence rates, but recent advances based on block LU factorization combined with multigrid for the resulting definite systems have led to preconditioners that deliver mesh-independent convergence rates.^[17]

SCOPE FOR FUTURE WORK

Various methods to solve problems of fluid mechanics using CFD have been discussed in brief but the comparison of various methods is not done till now. So this work is far from completion. Many comparative parameters may be designed in coming future so that these methods can be compared on the basis of these parameters and better methods can be found out.

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