

Computational Methods in Fluid Mechanics

A Handbook

Gabriel Alozondo
Editor

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Preface

Computational fluid dynamics, usually abbreviated as CFD, is a branch of fluid mechanics that uses numerical methods and algorithms to solve and analyse 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 yields software that improves the accuracy and speed of complex simulation scenarios such as transonic or turbulent flows. Initial experimental validation of such software is performed using a wind tunnel with the final validation coming in full-scale testing, e.g. flight tests. The fundamental basis of almost all CFD problems are the Navier–Stokes equations, which define any single-phase (gas or liquid, but not both) fluid flow. These equations can be simplified by removing terms describing viscous actions to yield the Euler equations. Further simplification, by removing terms describing vorticity yields the full potential equations. Finally, for small perturbations in subsonic and supersonic flows (not transonic or hypersonic) these equations can be linearized to yield the linearized potential equations. Historically, methods were first developed to solve the Linearized potential equations. Two-dimensional (2D) methods, using conformal transformations of the flow about a cylinder to the flow about an airfoil were developed in the 1930s. The computer power available paced development of three-dimensional methods. The first work using computers to model fluid flow, as governed by the Navier-Stokes equations, was performed at Los Alamos National Labs, in the T3 group. This group was led by Francis H. Harlow, who is widely considered as one of the pioneers of CFD. From 1957 to late 1960s, this group developed a variety of numerical methods to simulate transient two-dimensional fluid flows, such as Particle-in-cell method, Fluid-in-cell method, Vorticity stream function method, and Marker-and-cell method. Fromm's vorticity-stream-function method for 2D,

transient, incompressible flow was the first treatment of strongly contorting incompressible flows in the world.

The first paper with three-dimensional model was published by John Hess and A.M.O. Smith of Douglas Aircraft in 1967. This method discretized the surface of the geometry with panels, giving rise to this class of programs being called Panel Methods. Their method itself was simplified, in that it did not include lifting flows and hence was mainly applied to ship hulls and aircraft fuselages. The first lifting Panel Code (A230) was described in a paper written by Paul Rubbert and Gary Saaris of Boeing Aircraft in 1968. In time, more advanced three-dimensional Panel Codes were developed at Boeing (PANAIR, A502), Lockheed (Quadpan), Douglas (HESS), McDonnell Aircraft (MACAERO), NASA (PMARC) and Analytical Methods (WBAERO, USAERO and VSAERO). Some (PANAIR, HESS and MACAERO) were higher order codes, using higher order distributions of surface singularities, while others (Quadpan, PMARC, USAERO and VSAERO) used single singularities on each surface panel. The advantage of the lower order codes was that they ran much faster on the computers of the time. Today, VSAERO has grown to be a multi-order code and is the most widely used program of this class. It has been used in the development of many submarines, surface ships, automobiles, helicopters, aircraft, and more recently wind turbines. Its sister code, USAERO is an unsteady panel method that has also been used for modelling such things as high speed trains and racing yachts. The NASA PMARC code from an early version of VSAERO and a derivative of PMARC, named CMARC, is also commercially available.

This book aims at bridging the gap between the two streams above by providing the reader with the theoretical background of basic CFD methods without going into deep detail of the mathematics or numerical algorithms. This book provides the basics of Computational Fluid Dynamics appropriate to modern day undergraduate study. The aim is to bridge the gap between books focusing on detailed theoretical analysis and commercial software user's guides which do not contain significant theory.

—Editor

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Chapter 1

Introduction

Fluid Dynamics

In physics, fluid dynamics is a subdiscipline of fluid mechanics that deals with fluid flow—the natural science of fluids (liquids and gases) in motion. It has several subdisciplines itself, including aerodynamics (the study of air and other gases in motion) and hydrodynamics (the study of liquids in motion). Fluid dynamics has a wide range of applications, including calculating forces and moments on aircraft, determining the mass flow rate of petroleum through pipelines, predicting weather patterns, understanding nebulae in interstellar space and reportedly modelling fission weapon detonation. Some of its principles are even used in traffic engineering, where traffic is treated as a continuous fluid.

Fluid dynamics offers a systematic structure—which underlies these practical disciplines—that embraces empirical and semi-empirical laws derived from flow measurement and used to solve practical problems. The solution to a fluid dynamics problem typically involves calculating various properties of the fluid, such as velocity, pressure, density, and temperature, as functions of space and time.

Before the twentieth century, *hydrodynamics* was synonymous with fluid dynamics. This is still reflected in names of some fluid dynamics topics, like magnetohydrodynamics and hydrodynamic stability, both of which can also be applied to gases.

Equations of Fluid Dynamics

The foundational axioms of fluid dynamics are the conservation laws, specifically, conservation of mass, conservation of linear momentum (also known as Newton's Second Law of Motion), and

conservation of energy (also known as First Law of Thermodynamics). These are based on classical mechanics and are modified in quantum mechanics and general relativity. They are expressed using the Reynolds Transport Theorem.

In addition to the above, fluids are assumed to obey the *continuum assumption*. Fluids are composed of molecules that collide with one another and solid objects. However, the continuum assumption considers fluids to be continuous, rather than discrete. Consequently, properties such as density, pressure, temperature, and velocity are taken to be well-defined at infinitesimally small points, and are assumed to vary continuously from one point to another. The fact that the fluid is made up of discrete molecules is ignored.

For fluids which are sufficiently dense to be a continuum, do not contain ionized species, and have velocities small in relation to the speed of light, the momentum equations for Newtonian fluids are the Navier-Stokes equations, which is a non-linear set of differential equations that describes the flow of a fluid whose stress depends linearly on velocity gradients and pressure. The unsimplified equations do not have a general closed-form solution, so they are primarily of use in Computational Fluid Dynamics. The equations can be simplified in a number of ways, all of which make them easier to solve. Some of them allow appropriate fluid dynamics problems to be solved in closed form.

In addition to the mass, momentum, and energy conservation equations, a thermodynamical equation of state giving the pressure as a function of other thermodynamic variables for the fluid is required to completely specify the problem. An example of this would be the perfect gas equation of state:

$$p = \frac{\rho R_u T}{M}$$

where p is pressure, ρ is density, R_u is the gas constant, M is the molar mass and T is temperature.

Conservation Laws

Three conservation laws are used to solve fluid dynamics problems, and may be written in integral or differential form. Mathematical formulations of these conservation laws may be interpreted by considering the concept of a *control volume*. A control volume is a specified volume in space through which air can flow in and out. Integral formulations of the conservation laws consider the change

in mass, momentum, or energy within the control volume. Differential formulations of the conservation laws apply Stokes' theorem to yield an expression which may be interpreted as the integral form of the law applied to an infinitesimal volume at a point within the flow.

- **Mass continuity (conservation of mass):** The rate of change of fluid mass inside a control volume must be equal to the net rate of fluid flow into the volume. Physically, this statement requires that mass is neither created nor destroyed in the control volume, and can be translated into the integral form of the continuity equation:

$$\frac{\partial}{\partial t} \iiint_V \rho dV = - \iint_{S_{pu}} \rho \mathbf{u} \cdot d\mathbf{S}$$

Above, ρ is the fluid density, \mathbf{u} is a velocity vector, and t is time. The left-hand side of the above expression contains a triple integral over the control volume, whereas the right-hand side contains a double integral over the surface of the control volume. The differential form of the continuity equation is:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

- **Conservation of Momentum:** This equation applies Newton's second law of motion to the control volume, requiring that any change in momentum of the air within a control volume be due to the net flow of air into the volume and the action of external forces on the air within the volume. In the integral formulation of this equation, body forces here are represented by f_{body} , the body force per unit mass. Surface forces, such as viscous forces, are represented by \mathbf{F}_{surf} , the net force due to stresses on the control volume surface.

$$\frac{\partial}{\partial t} \iiint_V \rho \mathbf{u} dV = - \iint_{S(\rho \mathbf{u} \cdot d\mathbf{S})} \rho \mathbf{u} \cdot d\mathbf{S} + \iint_{S} \rho \mathbf{f}_{body} dV + \mathbf{F}_{surf}$$

The differential form of the momentum conservation equation is as follows. Here, both surface and body forces are accounted for in one total force, \mathbf{F} . For example, \mathbf{F} may be expanded into an expression for the frictional and gravitational forces acting on an internal flow.

$$\frac{D\mathbf{u}}{Dt} = \mathbf{F} - \frac{\nabla p}{\rho}$$

In aerodynamics, air is assumed to be a Newtonian fluid, which posits a linear relationship between the shear stress (due to internal

friction forces) and the rate of strain of the fluid. The equation above is a vector equation: in a three dimensional flow, it can be expressed as three scalar equations. The conservation of momentum equations for the compressible, viscous flow case are called the Navier-Stokes equations.

- Conservation of Energy: Although energy can be converted from one form to another, the total energy in a given closed system remains constant.

$$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} + \nabla \cdot (k \nabla T) + \Phi$$

Above, h is enthalpy, k is the thermal conductivity of the fluid, T is temperature, and Φ is the viscous dissipation function. The viscous dissipation function governs the rate at which mechanical energy of the flow is converted to heat. The second law of thermodynamics requires that the dissipation term is always positive: viscosity cannot create energy within the control volume. The expression on the left side is a material derivative.

Compressible vs Incompressible Flow

All fluids are compressible to some extent, that is, changes in pressure or temperature will result in changes in density. However, in many situations the changes in pressure and temperature are sufficiently small that the changes in density are negligible. In this case the flow can be modelled as an incompressible flow. Otherwise the more general compressible flow equations must be used.

Mathematically, incompressibility is expressed by saying that the density ρ of a fluid parcel does not change as it moves in the flow field, i.e.,

$$\frac{D\rho}{Dt} = 0,$$

where D/Dt is the substantial derivative, which is the sum of local and convective derivatives. This additional constraint simplifies the governing equations, especially in the case when the fluid has a uniform density.

For flow of gases, to determine whether to use compressible or incompressible fluid dynamics, the Mach number of the flow is to be evaluated. As a rough guide, compressible effects can be ignored at Mach numbers below approximately 0.3. For liquids, whether the incompressible assumption is valid depends on the fluid properties (specifically the critical pressure and temperature of the fluid) and

the flow conditions (how close to the critical pressure the actual flow pressure becomes). Acoustic problems always require allowing compressibility, since sound waves are compression waves involving changes in pressure and density of the medium through which they propagate.

Viscous vs Inviscid Flow

Viscous problems are those in which fluid friction has significant effects on the fluid motion.

The Reynolds number, which is a ratio between inertial and viscous forces, can be used to evaluate whether viscous or inviscid equations are appropriate to the problem.

Stokes flow is flow at very low Reynolds numbers, $Re \ll 1$, such that inertial forces can be neglected compared to viscous forces.

On the contrary, high Reynolds numbers indicate that the inertial forces are more significant than the viscous (friction) forces. Therefore, we may assume the flow to be an inviscid flow, an approximation in which we neglect viscosity completely, compared to inertial terms.

This idea can work fairly well when the Reynolds number is high. However, certain problems such as those involving solid boundaries, may require that the viscosity be included. Viscosity often cannot be neglected near solid boundaries because the no-slip condition can generate a thin region of large strain rate (known as Boundary layer) which enhances the effect of even a small amount of viscosity, and thus generating vorticity. Therefore, to calculate net forces on bodies (such as wings) we should use viscous flow equations. As illustrated by d'Alembert's paradox, a body in an inviscid fluid will experience no drag force. The standard equations of inviscid flow are the Euler equations. Another often used model, especially in computational fluid dynamics, is to use the Euler equations away from the body and the boundary layer equations, which incorporates viscosity, in a region close to the body.

The Euler equations can be integrated along a streamline to get Bernoulli's equation. When the flow is everywhere irrotational and inviscid, Bernoulli's equation can be used throughout the flow field. Such flows are called potential flows.

Steady vs Unsteady Flow

When all the time derivatives of a flow field vanish, the flow is considered to be a steady flow. Steady-state flow refers to the condition where the fluid properties at a point in the system do not change over

time. Otherwise, flow is called unsteady (also called transient). Whether a particular flow is steady or unsteady, can depend on the chosen frame of reference. For instance, laminar flow over a sphere is steady in the frame of reference that is stationary with respect to the sphere. In a frame of reference that is stationary with respect to a background flow, the flow is unsteady.

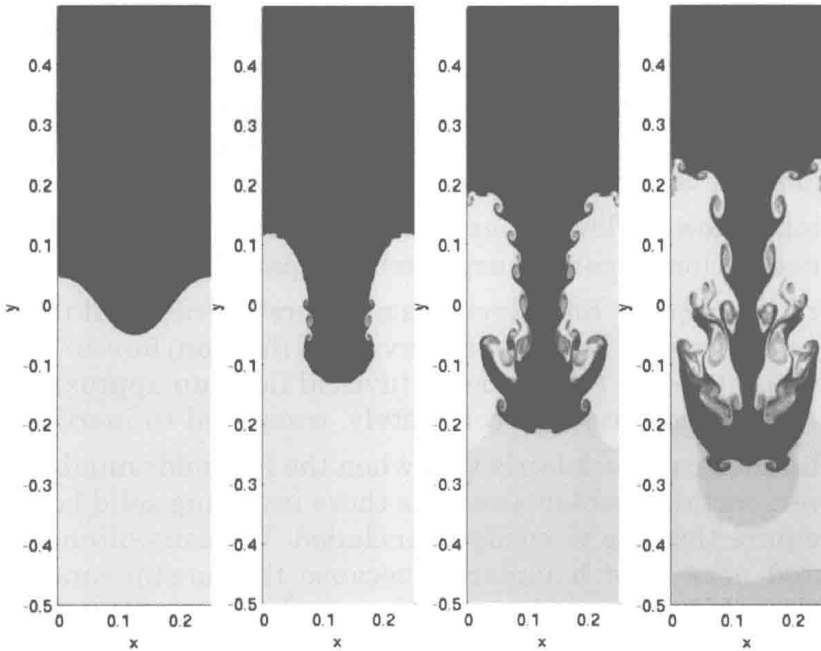


Figure: *Hydrodynamics simulation of the Rayleigh–Taylor instability*

Turbulent flows are unsteady by definition. A turbulent flow can, however, be statistically stationary. According to Pope:

The random field $U(x,t)$ is statistically stationary if all statistics are invariant under a shift in time.

This roughly means that all statistical properties are constant in time. Often, the mean field is the object of interest, and this is constant too in a statistically stationary flow.

Steady flows are often more tractable than otherwise similar unsteady flows. The governing equations of a steady problem have one dimension fewer (time) than the governing equations of the same problem without taking advantage of the steadiness of the flow field.

Laminar vs Turbulent Flow

Turbulence is flow characterized by recirculation, eddies, and apparent randomness. Flow in which turbulence is not exhibited is

called laminar. It should be noted, however, that the presence of eddies or recirculation alone does not necessarily indicate turbulent flow—these phenomena may be present in laminar flow as well. Mathematically, turbulent flow is often represented via a Reynolds decomposition, in which the flow is broken down into the sum of an average component and a perturbation component.

It is believed that turbulent flows can be described well through the use of the Navier–Stokes equations. Direct numerical simulation (DNS), based on the Navier–Stokes equations, makes it possible to simulate turbulent flows at moderate Reynolds numbers. Restrictions depend on the power of the computer used and the efficiency of the solution algorithm. The results of DNS have been found to agree well with experimental data for some flows.

Most flows of interest have Reynolds numbers much too high for DNS to be a viable option, given the state of computational power for the next few decades. Any flight vehicle large enough to carry a human ($L > 3$ m), moving faster than 72 km/h (20 m/s) is well beyond the limit of DNS simulation ($Re = 4$ million). Transport aircraft wings (such as on an Airbus A300 or Boeing 747) have Reynolds numbers of 40 million (based on the wing chord). In order to solve these real-life flow problems, turbulence models will be a necessity for the foreseeable future.

Reynolds-averaged Navier–Stokes equations (RANS) combined with turbulence modelling provides a model of the effects of the turbulent flow. Such a modelling mainly provides the additional momentum transfer by the Reynolds stresses, although the turbulence also enhances the heat and mass transfer. Another promising methodology is large eddy simulation (LES), especially in the guise of detached eddy simulation (DES)—which is a combination of RANS turbulence modelling and large eddy simulation.

Newtonian vs Non-Newtonian Fluids

Sir Isaac Newton showed how stress and the rate of strain are very close to linearly related for many familiar fluids, such as water and air. These Newtonian fluids are modelled by a coefficient called viscosity, which depends on the specific fluid.

However, some of the other materials, such as emulsions and slurries and some visco-elastic materials (e.g. blood, some polymers), have more complicated *non-Newtonian* stress-strain behaviours. These materials include *sticky liquids* such as latex, honey, and lubricants which are studied in the sub-discipline of rheology.

Subsonic vs Transonic, Supersonic and Hypersonic Flows

While many terrestrial flows (e.g. flow of water through a pipe) occur at low mach numbers, many flows of practical interest (e.g. in aerodynamics) occur at high fractions of the Mach Number $M=1$ or in excess of it (supersonic flows). New phenomena occur at these Mach number regimes (e.g. shock waves for supersonic flow, transonic instability in a regime of flows with M nearly equal to 1, non-equilibrium chemical behaviour due to ionization in hypersonic flows) and it is necessary to treat each of these flow regimes separately.

Magnetohydrodynamics

Magnetohydrodynamics is the multi-disciplinary study of the flow of electrically conducting fluids in electromagnetic fields. Examples of such fluids include plasmas, liquid metals, and salt water. The fluid flow equations are solved simultaneously with Maxwell's equations of electromagnetism.

Other Approximations

There are a large number of other possible approximations to fluid dynamic problems. Some of the more commonly used are listed below.

- The Boussinesq approximation neglects variations in density except to calculate buoyancy forces. It is often used in free convection problems where density changes are small.
- Lubrication theory and Hele-Shaw flow exploits the large aspect ratio of the domain to show that certain terms in the equations are small and so can be neglected.
- Slender-body theory is a methodology used in Stokes flow problems to estimate the force on, or flow field around, a long slender object in a viscous fluid.
- The shallow-water equations can be used to describe a layer of relatively inviscid fluid with a free surface, in which surface gradients are small.
- The Boussinesq equations are applicable to surface waves on thicker layers of fluid and with steeper surface slopes.
- Darcy's law is used for flow in porous media, and works with variables averaged over several pore-widths.
- In rotating systems, the quasi-geostrophic approximation assumes an almost perfect balance between pressure gradients