Introduction to Compressible Computational Fluid Dynamics

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Abstract

This document is intended as an introduction to computational fluid dynamics at the upper undergraduate level. It is assumed that the student has had courses through three dimensional calculus and some computer programming experience with numerical algorithms. A course in differential equations is recommended. This document is intended to be used by undergraduate instructors and students to gain an understanding of computational fluid dynamics. The document can be used in a classroom or research environment at the undergraduate level. The idea of this work is to have the students use the modules to discover properties of the equations and then relate this to the physics of fluid dynamics. Many issues, such as rarefactions and shocks are left out of the discussion because the intent is to have the students discover these concepts and then study them with the instructor. The document is used in part of the undergraduate MATH 365 - Computation Fluid Dynamics course at James Madison University (JMU) and is part of the joint NSF Grant between JMU and North Carolina Central University (NCCU): A Collaborative Computational Sciences Program.

This document introduces the full three-dimensional Navier Stokes equations. Assumptions to these equations are made to derive equations that are accessible to undergraduates with the above prerequisites. These equations are approximated using finite difference methods. The development of the equations and finite difference methods are contained in this document. Software modules and their corresponding documentation in Fortran 90, Maple and Matlab can be downloaded from the website: www.math.jmu./edu/ jim/compressible.html. The software modules and their corresponding documentation are mentioned in this document.

Introduction

Computational fluid dynamics (CFD) usually involves working with some form of the Navier-Stokes equations. These forms are usually obtained by making some assumptions that simplify the equations. The next step is to develop a numerical algorithm for solving these equations.

The Navier-Stokes equations are commonly expressed in one of two forms. One form is known as the incompressible flow equations and the other is known as the compressible flow equations. The incompressible flow equations model fluids whose density does not change over time. The compressible flow equations allow the density of the fluid to change with the flow.

This document will consider the compressible flow equations. The compressible Navier-Stokes equations are intimidating partial differential equations (PDE's) and rightfully so. They are extremely difficult mathematical equations that describe the motion of a fluid in three dimensions (3D). The equations allow for velocity changes, density changes, energy changes and viscous effects. To appreciate the complexity of these equations think about the flow of water down a rocky incline. These equations can be simplified by making some assumptions about the flow of the fluid that turns the problem into a two dimensional (2D) or sometimes a one dimensional (1D) problem.

The discussions in this document are meant to help you understand some of the complexities of the Navier-Stokes equations. Of course, there are whole industries working on these equations and no industry understands them completely. There are, of course, many mathematical questions that have not been answered regarding the full 3D Navier-Stokes equations.

If assumptions can be made about the fluid being studied the Navier-Stokes equations can be converted into 1D and 2D problems. Many mathematical properties are known about some of these 1D and 2D PDE's. You can study some of these PDE's numerically in the equation documents described in this work.

We now present the full 3D Navier-Stokes equations. The equations are obtained by applying Newton's force laws, the conservation of mass principle and conservation of energy principle to the motion of a fluid. In this document we will assume that you have seen this development in a physics course or have considered the modules at the James Madison University Computational Science site that develop these equations.

The (3D) Navier-Stokes equations are

[1] The Momentum Equation or The Momentum Balance Equation

$$\rho(\frac{\partial}{\partial t}\bar{u} + (\bar{u}\cdot\nabla)\bar{u}) + \nabla p - \delta\Delta\bar{u} - (\eta + \frac{1}{3}\mu)\nabla\nabla\cdot\bar{u} = \bar{g}$$

[2] The Continuity Equation or The Mass Balance Equation

$$\tfrac{\partial}{\partial t}\rho + \nabla\cdot(\rho\bar{u}) = 0$$

[3] The Energy Equations or The Energy Balance Equations

(E1) $\tfrac{\partial}{\partial t}\rho(\tfrac{1}{2}\bar{u}\cdot\bar{u} + \epsilon) + \nabla\cdot(\rho\bar{u}(\tfrac{1}{2}\bar{u}\cdot\bar{u} + \omega)) = 0$

(E2) $\tfrac{\partial}{\partial t}E + \nabla\cdot((E + p)\bar{u}) = 0$

[4] The Equations of State

(S1) $p = c^2\rho$ (Acoustics - sound waves)

(S2) $p = (\gamma - 1)(E - \tfrac{1}{2}\rho\bar{u}\cdot\bar{u})$ (Gas Dynamics)

(S3) $p = \alpha\rho^k$ (Gas Dynamics)

The momentum equation is really 3 equations since

$$\bar{u} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} u_1(x_1, x_2, x_3, t) \\ u_2(x_1, x_2, x_3, t) \\ u_3(x_1, x_2, x_3, t) \end{pmatrix}$$

or

$$\bar{u} = \begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} u(x, y, z, t) \\ v(x, y, z, t) \\ w(x, y, z, t) \end{pmatrix}.$$

Newton's force law is applied in all three dimensions. Since $\bar{u} = (u_1, u_2, u_3)$ or $\bar{u} = (u, v, w)$, the u_1 (or u) component is the velocity of the fluid in the x_1 (or x) direction, the u_2 (or v) component is the velocity of the fluid in the x_2 (or y) direction and the u_3 (or w) component is the velocity of the fluid in the x_3 (or z) direction. (We will use both of these notations for our space dimensions.) Under the energy equations we have listed two energy equations because both forms of these equations are commonly used. We have also listed some equations of state. The equations of state are experimentally derived equations and allow us to eliminate one of the unknowns so that we have 5 PDE's and 5 unknowns. That is, the (3D) Navier-Stokes equations are a system of 5 PDE's. In this document, the documents describing the software modules and the software modules will only use the energy equation (e2) and one of the two state equations (S1) or (S2). (In (E1) ϵ is the internal energy and ω is the enthalpy.)

We now explain the notation used in the Navier-Stoke's equations; $\rho = \rho(x, y, z, t)$ is the density of the fluid at a point (x, y, z) at time t, $p = p(x, y, z, t)$ is the pressure on the fluid at a point (x, y, z) at time t. The symbol ∇ represents the gradient (column) vector $(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3})$ or $(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})$. By ∇p we mean the (column) vector (p_x, p_y, p_z), where the subscript indicates partial differentiation with respect to that variable. The symbol Δ represents the Laplacian and is given by $\nabla \cdot \nabla$ or $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ and is applied to each component of $\bar{u} = (u, v, w)$. The parameters δ, η and μ are functions of (x, y, z) that describe the viscosity of the fluid. The function $\bar{g}$ is the (column) vector $(g_1(x, y, z, t), g_2(x, y, z, t), g_3(x, y, z, t))$ and models external forces acting on the fluid. In the modules we set $\bar{g} = \bar{0}$. You can easily modify the codes to see what effects external forces have on the fluid flow and the mathematical equations. The internal energy of the fluid is modeled by $\epsilon = \epsilon(x, y, z, t)$ and the total energy of the fluid is modeled by $E = E(x, y, z, t)$. The speed of sound in the fluid is given by $c = c(x, y, z)$. The functions c, α, k and γ are determined experimentally. In the software modules c, α, k and γ are constant.

THE EULER EQUATIONS

The Euler equations are obtained from the Navier-Stokes equations by assuming the fluid is viscous-free. Dropping these terms from the Navier-Stokes equations gives us the (3D) Euler equations

[1] Momentum Equation or Momentum Balance

$$\rho(\tfrac{\partial}{\partial t}\bar{u} + (\bar{u}\cdot\nabla)\bar{u}) + \nabla p = \bar{g}$$

[2] Continuity equation or Mass Balance

$$\tfrac{\partial}{\partial t}\rho + \nabla\cdot(\rho\bar{u}) = 0$$

[3] The Energy Equations or The Energy Balance Equations

(E1) $\quad \tfrac{\partial}{\partial t}\rho(\tfrac{1}{2}\bar{u}\cdot\bar{u} + \epsilon) + \nabla\cdot(\rho\bar{u}(\tfrac{1}{2}\bar{u}\cdot\bar{u} + w) = 0$

(E2) $\quad \tfrac{\partial}{\partial t}E + \nabla\cdot((E+p)\bar{u}) = 0$

[4] The Equations of State

(S1) $\quad p = c^2\rho$ (Acoustics - sound waves)

(S2) $\quad p = (\gamma - 1)(E - \tfrac{1}{2}\rho\bar{u}\cdot\bar{u})$ (Gas Dynamics)

(S3) $\quad p = \alpha\rho^k$ (Gas Dynamics)

As an exercise you should carry out the differentiation and vector operations in the Navier-Stokes and Euler equations and express the PDE's for these equations in terms of the components of $\bar{u}$ using either the

$$\bar{u} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} u_1(x_1,x_2,x_3,t) \\ u_2(x_1,x_2,x_3,t) \\ u_3(x_1,x_2,x_3,t) \end{pmatrix}$$

or

$$\bar{u} = \begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} u(x,y,z,t) \\ v(x,y,z,t) \\ w(x,y,z,t) \end{pmatrix}$$

notation.

THE 1D NAVIER-STOKES AND EULER EQUATIONS

In the modules we will only consider the (1D) equations. A study of the (1D) equations will give you an insight into the difficulties of studying fluid mechanics and of simulating fluid flow on a computer. Many of the problems arising in (1D) have to be considered in both (2D) and (3D). Of course, more problems arise in (2D) than (1D) and in (3D) than (2D). The modules are meant to give you an understanding of the complexities of computational science and of what computational science is and how it is used in CFD. Although, we are studying fluid flow the ideas of developing a system of equations that describe a phenomena, numerically approximating these equations and their solutions with algorithms, using computers to run the algorithms and using computers to visualize the results make up computational science. Of course, studying each of these steps and the difficulties of each step also make up computational science.

A physical interpretation of the 1D equations is to think of the flow of a fluid in a thin tube or a narrow channel and how the properties of the fluid; velocity, density and energy change only along the tube or the channel. Of course, problems like this occur all the time. Drinking straws, ditches and blood veins are some examples.

We will write the (1D) Navier-Stokes equations as

[1] The Momentum Equation or The Momentum Balance Equation

$$\rho(\tfrac{\partial}{\partial t}u + u\tfrac{\partial}{\partial x}u) + \tfrac{\partial}{\partial x}p - \delta\tfrac{\partial^2}{\partial x^2}u - (\eta + \tfrac{1}{3}\mu)\tfrac{\partial^2}{\partial x^2}u = g(x,t)$$

[2] The Continuity Equation or The Mass Balance Equation

$$\tfrac{\partial}{\partial t}\rho + \tfrac{\partial}{\partial x}(\rho u) = 0$$

[3] The Energy Equation or The Energy Balance Equation

$$\frac{\partial}{\partial t}E + \frac{\partial}{\partial x}((E+p)u) = 0$$

[4] The Equations of State

(S1) $p = c^2\rho$ (Acoustics - sound waves)

(S2) $p = (\gamma - 1)(E - \tfrac{1}{2}\rho u^2)$ (Gas Dynamics)

Note that the momentum equation can be written as

$$\rho u_t + \rho u u_x + p_x - \alpha u_{xx} = g$$

or

$$\rho(u_t + (\tfrac{1}{2}u^2)_x) + p_x - \alpha u_{xx} = g$$

where $\alpha = \delta + \eta + \frac{1}{3}\mu$. If the pressure does not depend on x this equation reduces to

$$\rho(u_t + uu_x) - \alpha u_{xx} = g$$

or

$$\rho(u_t + (\tfrac{1}{2}u^2)_x) - \alpha u_{xx} = g.$$

Now suppose the fluid density, ρ is a constant. Dividing by ρ gives us

$$\text{(B1)} \qquad u_t + uu_x - \nu u_{xx} = G$$

or

$$\text{(B2)} \qquad u_t + (\tfrac{1}{2}u^2)_x - \nu u_{xx} = G.$$

where $\nu = \frac{\alpha}{\rho}$ and $G(x,t) = \frac{g(x,t)}{\rho}$. These PDE's are known as Burger's equation with viscosity. Equation (B1) is known as the non-conservation form of Burger's equation and equation (B2) is known as the conservation form of Burger's equation. A study of these equations will help you to understand fluid velocity in the Navier-Stokes equations. You can click on the Burger's Modules Description Document link to learn how to do a numerical study of these equations through the software modules. A good discovery project is to modify the modules to include viscosity and then study what happens as $\nu \to 0$ and compare this with the numerical solution to Burger's equation with $\nu = 0$. After this study return to equation (B2) and see how you could verify your numerical results analytically.

We now consider the Continuity Equation PDE. If the fluid velocity u is a constant this PDE reduces to

$$\text{(W)} \qquad \tfrac{\partial}{\partial t}\rho + u\tfrac{\partial}{\partial x}(\rho) = 0.$$

We leave it as an exercise for you to use the chain rule of differentiation to show that $\rho(x,t) = f(x-ut)$ is a general solution to this PDE for an arbitrary differentiable function f and a constant fluid velocity u. Note that $\rho(x,0) = f(x)$. Therefore, physically f is the fluid density at time 0 or the initial fluid density. Also, note that the graph of $f(x-ut)$ is a translation of the graph of $f(x)$ to the right or left by a distance $|ut|$ depending on the sign of u. Therefore, the general solution to equation (W) is a translation of the initial density by $|ut|$. We see that over time the initial density moves to the right or left by an amount $|ut|$. That is, as the time t increases the initial density moves further to the right or to the left. This is known as a wave. Since $|ut|$ can be thought of as the distance the initial density moves, we will call $|u|$ the speed of the wave. To do a numerical study of advection diffusion equation click on the Advection Diffusion Modules Description Document link. This document will describe the software modules for this equation. You will observe the phenomena described above in these software modules.

Note that equation (B1) and equation (W) are similar to the PDE

$$\text{(AD)} \qquad w_t + cw_x + dw_{xx} = h(x,t).$$

This PDE is known as the advection-diffusion equation. In order to get (B1) from (AD) we replace u by w in the partial derivative expressions, u with no derivatives by c and α by d. In order to get (W) from (AD) we replace ρ by w, u by c and d would equal 0. In the software modules you will see that c is the speed (or advection) of the wave and d is the diffusion of the system.

We now consider the (1D) Euler equations. An understanding of these equations is essential to understanding the (1D) Navier-Stokes equations. After completing the modules associated with the (1D) Euler equations you should be able to write your own codes for the (1D) Navier-Stokes equations.

The (1D) Euler equations which we will denote as (E1) are

[1] The Momentum Equation or The Momentum Balance Equation

$$\rho(\tfrac{\partial}{\partial t}u + u\tfrac{\partial}{\partial x}u) + \tfrac{\partial}{\partial x}p = g(x,t)$$

[2] The Continuity Equation or The Mass Balance Equation

$$\tfrac{\partial}{\partial t}\rho + \tfrac{\partial}{\partial x}(\rho u) = 0$$

[3] The Energy Equation or The Energy Balance Equation

$$\frac{\partial}{\partial t}E + \frac{\partial}{\partial x}((E+p)u) = 0$$

[4] The Equations of State

$$\text{(S1)} \qquad p = c^2\rho \qquad \text{(Acoustics - sound waves)}$$

(S2) $p = (\gamma - 1)(E - \frac{1}{2}\rho u^2)$ (Gas Dynamics)

We now consider another form of the (1D) Euler equations. From the product rule we have that

$$(\rho u)_t = \rho_t u + \rho u_t$$

and that

$$\rho u_t = (\rho u)_t - \rho_t u.$$

From the continuity equation we have that $-\rho_t = \frac{\partial}{\partial x}(\rho u)$. Using this in the last equation we obtain

$$\rho u_t = (\rho u)_t + u\frac{\partial}{\partial x}(\rho u).$$

Substituting this into the momentum equation we see that

$$\begin{gathered} \rho u_t + \rho u\frac{\partial}{\partial x}u + \frac{\partial}{\partial x}p = \\ (\rho u)_t + u\frac{\partial}{\partial x}(\rho u) + \rho u\frac{\partial}{\partial x}u + \frac{\partial}{\partial x}p = \\ (\rho u)_t + \frac{\partial}{\partial x}(u\rho u) + \frac{\partial}{\partial x}p = g \end{gathered}$$

where in the last equality we used the product rule. From the last line we now obtain the following form for the momentum equation

$$(\rho u)_t + \frac{\partial}{\partial x}(u^2\rho + p) = g.$$

Using this form of the momentum equation the (1D) Euler equations (with this momentum equation) which we will denote as (E2) are

[1] The Momentum Equation or The Momentum Balance Equation

$$\tfrac{\partial}{\partial t}(\rho u) + \tfrac{\partial}{\partial x}(u^2\rho + p) = g$$

[2] The Continuity Equation or The Mass Balance Equation

$$\tfrac{\partial}{\partial t}\rho + \tfrac{\partial}{\partial x}(\rho u) = 0$$

[3] The Energy Equation or The Energy Balance Equation

$$\frac{\partial}{\partial t}E + \frac{\partial}{\partial x}((E+p)u) = 0$$

[4] The Equations of State

(S1) $p = c^2\rho$ (Acoustics - sound waves)

(S2) $p = (\gamma - 1)(E - \frac{1}{2}\rho u^2)$ (Gas Dynamics)

If we use (S1) in the momentum equation and the continuity equation we obtain the following system of equations for u and ρ which we will denote as (E3)

[1] The Momentum Equation or The Momentum Balance Equation

$$\tfrac{\partial}{\partial t}(\rho u) + \tfrac{\partial}{\partial x}((u^2 + c^2)\rho) = g$$

[2] The Continuity Equation or The Mass Balance Equation

$$\tfrac{\partial}{\partial t}\rho + \tfrac{\partial}{\partial x}(\rho u) = 0$$

or the following system of equations for u and p which we will denote as (E4)

[1] The Momentum Equation or The Momentum Balance Equation

$$\tfrac{\partial}{\partial t}(\tfrac{p}{c^2}u) + \tfrac{\partial}{\partial x}(\tfrac{u^2+c^2}{c^2}p) = g$$

[2] The Continuity Equation or The Mass Balance Equation

$$\tfrac{\partial}{\partial t}\tfrac{p}{c^2} + \tfrac{\partial}{\partial x}(\tfrac{p}{c^2}u) = 0$$

Since the speed of sound in the fluid is usually known, we see that both of these forms are two equations in two unknowns. We leave it as an exercise for you to show that these two equations can be written in the form

$$\frac{\partial}{\partial t}v_1 + \frac{\partial}{\partial x}f_1(v_1, v_2) = g(x)$$
$$\frac{\partial}{\partial t}v_2 + \frac{\partial}{\partial x}f_2(v_1, v_2) = 0.$$

(You need to determine v_1, v_2, f_1 and f_2.) Equations of this form are called conservation equations. You will find that the functions f_1 and f_2 are similar for (E3) and (E4). If you solve (E3) you can get the pressure from $p = c^2\rho$ and if you solve (E4) you can get the density from this same relationship. The software modules allow you to do a numerical study of equation (E3). To learn how to do this study click on the link One Dimensional Density Velocity Equations Modules Description Document. This document will describe the software modules dealing with this equation. Later, we will use the acoustic condition S2 ($p = c^2\rho$) to generate a linear equation for pressure disturbances.

If we use (S2) in the energy equation we obtain the following system of equations for u, ρ and E which we will denote as (E5)

[1] The Momentum Equation or The Momentum Balance Equation

$$\tfrac{\partial}{\partial t}(\rho u) + \tfrac{\partial}{\partial x}((\gamma - 1)(E - \tfrac{1}{2}\rho u^2)) = g$$

[2] The Continuity Equation or The Mass Balance Equation

$$\tfrac{\partial}{\partial t}\rho + \tfrac{\partial}{\partial x}(\rho u) = 0$$

[3] The Energy Equation or The Energy Balance Equation

$$\frac{\partial}{\partial t}E + \frac{\partial}{\partial x}((\gamma E - \frac{(1-\gamma)}{2}\rho u^2)u) = 0$$

Note these equations can be put in the form

$$\begin{aligned} \frac{\partial}{\partial t}v_1 + \frac{\partial}{\partial x}f_1(v_1, v_2, v_3) = 0 \\ \frac{\partial}{\partial t}v_2 + \frac{\partial}{\partial x}f_2(v_1, v_2, v_3) = 0 \\ \frac{\partial}{\partial t}v_3 + \frac{\partial}{\partial x}f_3(v_1, v_2, v_3) = 0 \end{aligned}$$

where $v_1 = (\rho u), v_2 = \rho$ and $v_3 = E$ and where

$$\begin{aligned} f_1(v_1, v_2, v_3) &= \tfrac{v_1^2}{v_2} + (\gamma - 1)(v_3 - \tfrac{1}{2}\tfrac{v_1^2}{v_2}) \\ f_2(v_1, v_2, v_3) &= v_1 \\ f_3(v_1, v_2, v_3) &= (\gamma v_3 - \tfrac{(1-\gamma)}{2}\tfrac{v_1^2}{v_2})\tfrac{v_1}{v_2} \end{aligned} .$$

We leave it as an exercise for you to carry out the process we did to get these conservation equations from (E1) and (S2) to get the conservation equation form for the (3D) Euler equations. To do a numerical study of the (1D) Euler equations click on the link One Dimensional Euler Equations Modules Description Document. This document will describe the software modules associated with this equation.

We could have substituted (S1) or (S2) directly into (E1) and used these equations in the modules. We leave this as an exercise for you. You can compare and contrast your codes for these systems with the codes in the modules.

The 1D Linearized Pressure Equation or Acoustic Equation

We will assume c is a constant in our derivation. To model the propagation of sound (acoustic or pressure) waves we will linearize the following two equations.

[1] The Momentum Equation or The Momentum Balance Equation

$$\tfrac{\partial}{\partial t}(\tfrac{p}{c^2}u) + \tfrac{\partial}{\partial x}(u^2 \tfrac{p}{c^2} + p) = 0$$

[2] The Continuity Equation or The Mass Balance Equation

$$\tfrac{\partial}{\partial t}\tfrac{p}{c^2} + \tfrac{\partial}{\partial x}(\tfrac{p}{c^2}u) = 0.$$

In acoustic (sound) waves the particle velocity u is small. That is, $|u| << 1$ implying $u^2 << u$. Therefore, we linearize the Momentum Equation by dropping the nonlinear terms containing u^2. This gives us

[1] The Momentum Equation or The Momentum Balance Equation

$$\tfrac{\partial}{\partial t}(\tfrac{p}{c^2}u) + \tfrac{\partial}{\partial x}p = 0$$

[2] The Continuity Equation or The Mass Balance Equation

$$\tfrac{\partial}{\partial t}\tfrac{p}{c^2} + \tfrac{\partial}{\partial x}(\tfrac{p}{c^2}u) = 0.$$

We differentiate the Momentum Equation with respect to x and the Continuity Equation with respect to t and equate the mixed partial derivative term $(\frac{p}{c^2}u)_{xt}$ to get

$$\text{(LP)} \qquad p_{tt} - c^2 p_{xx} = 0.$$

We leave it for you to show that

$$p(x,t) = f(x - ct) + g(x + ct)$$

for arbitrary functions f and g is a solution to (LP). That is, the linearized pressure equation has solutions made up waves traveling to the left and to the right with speed c.