Chapter 3

Governing Equations

3.1 Introduction

The governing equations are basically a set of equations which model a physical phenomena. In our context, they will be a set of partial differential equations (PDEs), also called system of PDEs. These equations define how different properties of interest vary within space and time. The properties of interest are called the dependent variables; and the space and time are called independent variables. The space is spanned by three mutually perpendicular axis denoted by the variables x, y, z and the variable for time is t. Choosing an origin point in space time and arbitrary values for variables x, y, z and t, the complete three dimensional space and time can be spanned. When we talk about solving the governing equations we need to restrict ourselves within a well defined bounded region in space and time. This is called the solution space. At the boundary of solution space we have to define additional conditions to obtain unique solutions.

The dependent variables are properties like pressure, density, temperature, velocity etc. The distribution of these properties is the solution that we are interested in for, say, designing a product or understanding the physics. The system of PDEs is said to be closed when the number of dependent variables are equal to the number of equations. In many cases, the number of equations are lesser than the number of dependent variables. We have to then use models relating different properties, thus adding more equations, to close the system of governing equations. These models are mostly based on empirical relations or simplified assumptions.

3.2 Generic form of system of PDEs

The governing PDEs used for simulation of various physical processes can be cast into a generic form,

$$\frac{\partial W}{\partial t} + \frac{\partial F_C}{\partial x} + \frac{\partial G_C}{\partial y} + \frac{\partial H_C}{\partial z} = \frac{\partial F_D}{\partial x} + \frac{\partial G_D}{\partial y} + \frac{\partial H_D}{\partial z} + S. \tag{3.1}$$

Here, W is called the "conservative variable vector" or simply "conservative vector". It is named so because the variables in this vector are an outcome of application of conservation laws. The vectors F_C, G_C and H_C are called the "convective flux vectors". They are named so because they contain the product of velocity with terms from conservative vector. Therefore capturing the phenomena of translation of conserved quantities due to convection currents. Most importantly, the convective flux vector does not contain any terms with space derivatives and is purely a function of the conservative vector. The vectors F_D, G_D and H_D are called the "diffusion flux vectors". All the terms with space derivatives are placed in these vectors. The diffusion flux vector is called so due to the fact that the spatial derivatives cause spreading (diffusion) or concentration of the quantities, even when the bulk fluid velocity is zero. The vector S is called the "source vector". All the remaining terms in the governing equation, which can be integrated over finite control spatial volume, are clubbed together in this vector. Take a look at the example PDEs in section 3.5 to have a better understanding of these terms.

In many practical applications the solution at the steady state is sought, which implies that the time derivative term tends to zero. In such applications, solving time accurate PDEs is unnecessary and probably inefficient. We may therefore, include an additional artificial time derivative term which can be tweaked for efficient computations. The governing equations therefore becomes,

$$\frac{\partial U}{\partial \tau} + \frac{\partial W}{\partial t} + \frac{\partial F_C}{\partial x} + \frac{\partial G_C}{\partial y} + \frac{\partial H_C}{\partial z} = \frac{\partial F_D}{\partial x} + \frac{\partial G_D}{\partial y} + \frac{\partial H_D}{\partial z} + S. \tag{3.2}$$

Here, τ is called the artificial or pseudo time variable and t is the real time variable. The vector U is called the artificial or pseudo conservative vector and to distinguish from this vector, W is now onwards called the real conservative vector. The units of U and W are the same, however the actual terms may be completely different. It is a common practice to write $U = PW$, where P is a pre conditioner introduced to make the numerical calculations efficient and accurate. The flux and source vectors are functions of the artificial conservative vector. For steady state simulations the term $\partial W/\partial t = 0$ and for unsteady simulations $\partial W/\partial t \neq 0$. In both the cases (steady and unsteady simulations), the term $\partial U/\partial \tau$ must tend to zero for accepting the computational result.

There is another minor detail worth mentioning for the reason of completeness. The form in which the equations are written above is called the "conservative form", not to be confused with the conservative vector. In this form, the flux vectors have all the variables inside the derivative, with no coefficients outside. The conservative form naturally arises when deriving the PDEs using conservation principles and applying the Gauss's theorem. This form is important for using the finite volume method, which will be explained in a later chapter. The advantage of writing the governing equations in a generic form is that now it is possible to discuss the various CFD techniques in a well defined setting. Also, this approach makes it possible to define computational models and write efficient computer programs which cater to a wide variety of applications which fit within this generic form.

3.3 Different types of variables

The variables in the conservative vector (called "conservative variables") are generally not very intuitive to us humans. Instead, we like to deal with quantities that we can measure and have a feel for. For example, the quantity – density multiplied by velocity – in the momentum equation is difficult to interpret, but we understand density and velocity separately. The so called "primitive variables" are introduced for this purpose. When we provide the inputs to the program or get outputs from the program, it is easier to deal with primitive variables.

The method of lines is a technique which is extensively used in the solution of time dependent PDEs. In this method it is useful to work with the so called "characteristics variables". Even though in computer programs we do not very often use these variables, they form the basis of many CFD techniques. Also in some boundary conditions, such as non reflective outlet boundary condition, the characteristics variables play an important role. When we say that we are solving the governing PDEs, it basically means that we are solving for the above mentioned dependent variables in space and time with specified boundary and/or initial conditions.

3.4 Representation of governing equations in code

When writing a computer program for solving the PDEs in question, we need to first find a way to represent them in the code. The way in which we represent the equations must be generic and efficient. As discussed above the variables may be needed in different forms at various places in the code and hence require conversion between them. This needs to be incorporated in the code through functions,

$$U \to W, \quad U \to V, \quad V \to U \quad \text{with} \quad U, W, V \in \mathbb{R}^N, \tag{3.3}$$

where, V is the vector of primitive variables. U and W are the artificial and real conservative variables respectively, as described earlier, and N is the number of PDEs in the governing equations. In addition to the above, the variables names will be needed for input and output formatting. The convective flux and the source vector can be described easily in terms of the artificial conservative vector U and therefore we can define functions for them as,

$$U \to (F_C, G_C, H_C), \quad U \to S \quad \text{with} \quad U, F_C, G_C, H_C, S \in \mathbb{R}^N. \tag{3.4}$$

The definition of functions for the diffusion flux vector requires not only the vector U, but also spatial derivatives. Hence, it is not very straightforward to define it in a generic code efficiently. This can be accomplished very elegantly using functional programming and lazy evaluations. This part of the text will be written once these concepts have been explained in context of object oriented programming in a later chapter.

Also, the characteristics of the convective flux and the material properties are necessary for the complete definition of the governing equations. There will also be some special cases when additional constitutive relations will be needed. All the above will be incorporated into the code by using an interface (abstract class). Hence making it extremely simple to adapt to any physical PDEs expressed in the generic form of the governing equations (3.2).

3.5 Few common governing equations

TODO

Navier Stokes
Euler
Stokes
shallow water
Axi symmetric flow
1D area varying nozzle
artificial compressibility
Incompressible with and without heat transfer
multiphase flow
Turbulence
Chemical reaction
Road traffic
Electromagnetism

3.6 Important properties of physical PDEs

TODO

Rotational invariance of system of PDEs
Homogeneity of flux function
Physical bounds on solutions