1. Introduction

Computational physics $\Longleftrightarrow$ Formulation of and numerical solution of large mechanical systems.

Mechanics is meant here as the science that quantitatively describes the motion, or tendency to motion, of material objects or systems of objects

Often, although the principles and even the basic equations of interesting systems are well established, they are in effect unsolved and little understood. In most problems, direct solutions by analysis prove impossible.

"A physical theory is a system of mathematical propositions, deduced from a small number of principles, which aim to present as simply, as exactly, and as completely as possible, a set of experimental laws" (Duhem, 1954)

What role does or can the computer have in the development of a physical theory?

The computer can provide the means by which we relate mathematical propositions to experimental laws. Each arithmetic operation performed by the computer is in itself no different from a calculation with a set of tables or a slide rule. It is because of the number of these operations that the computational medium of the computer offers is a new approach.

Scope and limitations of mathematical analysis and computational physics and their interactions with experiments.

Mathematical analysis $\Longleftrightarrow$ resolution by conventional algebraic methods, of physical principles to describe experimentally observed phenomena

* Has been very successful when the theory is linear, when symmetry can be invoked and when using only a few variables. ~~Better~~ Effective in describing continuous media.

* On the other hand, in computational physics, the mathematical properties of linearity, symmetry and a small number of variables are not demanded. The essence of the systems which may be described is that they have to be finite and discrete. Effective in describing many variable systems.

The three approaches are complementary, each of them can contribute to our understanding of a phenomena

[Mathematical analysis
Computational physics
Experiments

Computational physics $\Rightarrow$ can provide information when experiments is not possible

study of stars, ocean, relativity

However, Analytical or numerical models are only models and must continually be checked with the natural world through experiments.

$\Longrightarrow$ Application to Fluid Dynamics

Discretization

The central process in CFD is the process of discretization, i.e. the process of taking differential equations with an *infinite* number of degrees of freedom, and reducing it to a system of *finite* degrees of freedom. Hence, instead of determining the solution everywhere and for all times, we will be satisfied with its calculation at a finite number of locations and at specified time intervals. The partial differential equations are then reduced to a system of algebraic equations that can be solved on a computer.

Errors creep in during the discretization process. The nature and characteristics of the errors must be controlled in order to ensure that 1) we are solving the correct equations (consistency property), and 2) that the error can be decreased as we increase the number of degrees of freedom (stability and convegence). Once these two criteria are established, the power of computing machines can be leveraged to solve the problem in a numerically reliable fashion.

Various discretization schemes have been developed to cope with a variety of issues. The most notable for our purposes are: finite difference methods, finite volume methods, finite element methods, and spectral methods.

1.2.1 Finite Difference Method

Finite difference replace the infinitesimal limiting process of derivative calculation

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x} \tag{1.1}$$

with a finite limiting process,i.e.

$$f'(x) \approx \frac{f(x + \Delta x) - f(x)}{\Delta x} + O(\Delta x) \tag{1.2}$$

The term $O(\Delta x)$ gives an indication of the magnitude of the error as a function of the mesh spacing. In this instance, the error is halfed if the grid spacing, Δx is halved, and we say that this is a first order method. Most FDM used in practice are at least second order accurate except in very special circumstances. We will concentrate mostly on finite difference methods since they are still among the most popular numerical methods for the solution of PDE's because of their simplicity, efficiency, low computational cost, and ease of analysis. Their major drawback is in their geometric inflexibility which complicates their applications to general complex domains. These can be alleviated by the use of either mapping techniques and/or masking to fit the computational mesh to the computational domain.

1.2.2 Finite Element Method

The finite element method was designed to deal with problem with complicated computational regions. The PDE is first recast into a variational form which essentially forces the mean error to be small everywhere. The discretization step proceeds by dividing the computational domain into elements of triangular or rectangular shape. The solution within each element is interpolated with a polynomial of usually low order. Again, the unknowns are the solution at the collocation points. The CFD community adopted the FEM in the 1980's when reliable methods for dealing with advection dominated problems were devised.

1.2.3 Spectral Methods

Both finite element and finite difference methods are low order methods, usually of 2nd-4th order, and have local approximation property. By local we mean that a particular collocation point is affected by a limited number of points around it. In contrast, spectral method have global approximation property. The interpolation functions, either polynomials or trigonomic functions are global in nature. Their main benefits is in the rate of convergence which depends on the smoothness of the solution (i.e. how many continuous derivatives does it admit). For infinitely smooth solution, the error decreases exponentially, i.e. faster than algebraic. Spectral methods are mostly used in the computations of homogeneous turbulence, and require relatively simple geometries. Atmospheric model have also adopted spectral methods because of their convergence properties and the regular spherical shape of their computational domain.

1.2.4 Finite Volume Methods

Finite volume methods are primarily used in aerodynamics applications where strong shocks and discontinuities in the solution occur. Finite volume method solves an integral form of the governing equations so that local continuity property do not have to hold.

1.2.5 Computational Cost

The CPU time to solve the system of equations differ substantially from method to method. Finite differences are usually the cheapest on a per grid point basis followed by the finite element method and spectral method. However, a per grid point basis comparison is a little like comparing apple and oranges. Spectral methods deliver more accuracy on a per grid point basis than either FEM or FDM. The comparison is more meaningfull if the question is recast as "what is the computational cost to achieve a given error tolerance?". The problem becomes one of defining the error measure which is a complicated task in general situations.