3.1 Introduction

Any fluid flow is governed by three fundamental conservation laws, i.e., conservation of mass, conservation of momentum and conservation of energy. Governing equations for fluid flow are derived from the mathematical formulation of these laws. These governing equations are either in the form of partial differential equations or integral equations.

Partial differential equations are obtained if the governing equations are applied to an infinitesimal fluid particle moving within the flow, whereas the integral form of the governing equations is applied if the conservation laws are applied to a fixed volume in the flow domain. The equations are coupled and nonlinear in either of the cases, which can then be solved.

The governing equations are solved approximately on the computer using the software in computational fluid dynamics or CFD. The overview of this black box model is presented in Fig. 3.1. The CFD software converts the governing equations to a large set of algebraic equations using numerical methods. The large set of algebraic equations is inverted to get the cell center values. With recent advances in CFD technology, flow around realistic geometries and complex physics can be handled, thus saving project cost and time.

The CFD software used in this present study will be ANSYS Fluent from ANSYS Incorporated, a leading, general-purpose CFD solver used in the industry.

ANSYS Fluent solves the governing equations for fluid flow using a numerical technique called the finite volume method (FVM).

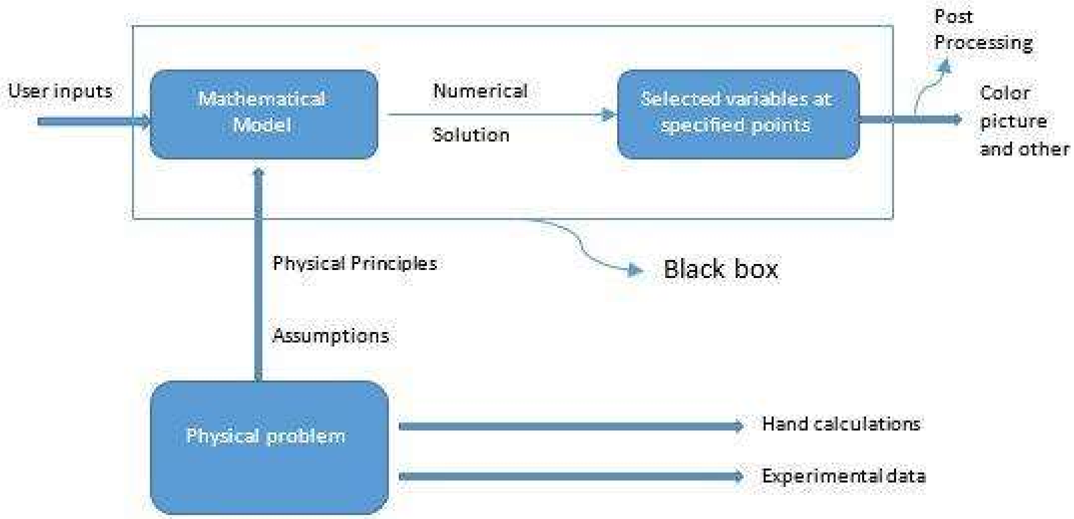

Figure 3. 1 Overview of Black Box Model (Courtesy of A Hands-on Introduction to Engineering Simulations (edX) by Dr.Rajesh Bhaskaran)

FVM technique allows the entire flow domain in a large number of small control volumes. The conservation equations are applied in these control volumes using the integral form of the governing equations, giving us a set of algebraic equations.

The Finite Volume Method (FVM) is preferred in CFD applications over the Finite element method (FEM) because the conservation equations are applied directly rather than indirectly. The quantities in each control volume are conserved in a discreet sense.

The numerical methodology of solving a problem consists of creating a mathematical model with assigned governing equations and boundary conditions.

3.2 Mathematical model

Flow-through a weir is unsteady in nature. A half key 3D PKW model has been used throughout the Thesis with the geometry of the physical experimental models.

The mathematical model consists of governing equations and boundary conditions, which are discussed below.

3.3 Governing Equations

ANSYS FLUENT solves mass, momentum and energy conservation equations for all flows. The governing equations are depicted in Table 3.1 below.

Table 3. 1 Conservation of mass and momentum equations

Sl. No.		Differential form	Integral form
1.	Conservation of mass	$\nabla.\vec{V} = 0$	$\int_S \vec{V} \cdot \hat{n}\, dS = 0$
2.	Conservation of Momentum	$\rho(\vec{V} \cdot \nabla)\vec{V} = -\nabla\rho + \mu\nabla^2\vec{V}$	$\int_S \rho\vec{V}(\vec{V} \cdot \hat{n})\, ds = \int_S p\, \hat{n}\, ds + \vec{F}_{visc}$

The first equation is the conservation of mass or the continuity equation. The law of mass conservation implies that the volume of a fluid particle moving within the flow cannot change or the net volume flow out of any arbitrary control volume has to be zero.

The second equation is the conservation of momentum, which represents the net pressure force on an infinitesimal fluid particle. It represents the net viscous friction or viscous shear on the infinitesimal fluid particle per unit volume. The governing equations are defined in a particular domain of the mathematical model in the present study.

3.4 Boundary conditions

The boundary conditions are defined at the edges of the domain. The simulations in the present study were performed on a 20 core CPU with the use of a parallel solver option and double precision. Half PKW unit was used to model the flow in a channel, the channel dimensions being the one used in the experimental study. The boundary conditions used in the present study are depicted in Fig. 3.2 below. The water inlet boundary was located at a sufficient distance (~ 19 P) for developing uniform flow conditions for the above numerical study.

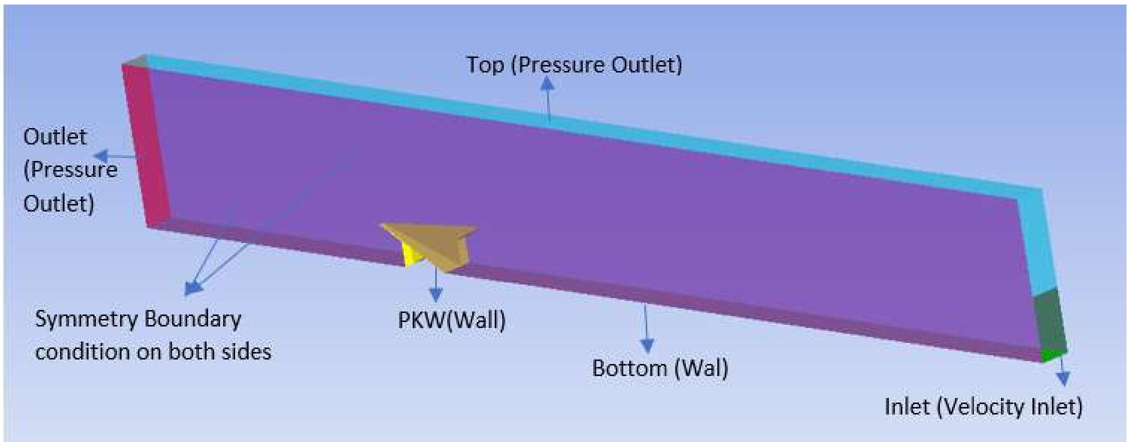

Figure 3. 2 Boundary condition of mathematical models

The wall boundary condition was used for PKW and bottom wall while the inlet was kept as velocity-inlet. Volume fraction at the inlet was specified as water being one and air being zero. The wall boundary was given a no-slip boundary condition, while the standard wall surface function was used to model the areas near the wall. The top portion of the channel and outlet portion was given a pressure outlet condition with no backflow of water. The sides of the channel were given a symmetry boundary condition. The mathematical model after assigning the governing equations and boundary conditions is complete.

3.5 Discretization Error and Numerical Solution Strategy

The mathematical model using the FVM in ANSYS Fluent requires splitting our domain into multiple control volumes or cells. FVM uses the integral form of these governing equations rather than the differential form.

The governing equations are satisfied in each cell of the domain, and the values of unknowns are determined at the cell centers of each cell. Discretization means determining unknown functions of selected variables at these selected points. The problem at hand thus reduces to finding cell center values to a fixed number of cell centers.

The cell centers values obtained as such are interpolated to get values at control surfaces, while boundary conditions (BCs) are provided at the edge of the domain of the control volume. Each of these algebraic equations relates a cell center value to its neighbors, and these algebraic equations are solved by inverting it on the computer to get the cell center values of unknowns we want to find.

This averaging and interpolation of the cell center values to get values at control surfaces introduces an error in this process. The error introduced in going from the integral form to the set of algebraic equations is called the discretization error. This discretization error can be reduced by using more cells in the domain, i.e., mesh refinement or increasing the order of accuracy of the interpolation.

Though the conservation is guaranteed in FVM, but there are interpolation errors which is unavoidable. But even on a coarse mesh, like this, the interpolation errors don't lead to spurious nonphysical results, such as mass accumulating or mass disappearing from a control volume or mass leaving a control volume doesn't match the mass entering the adjoining control volume, which could be the case in the finite element method.

The control volume balance for mass and momentum helps derive a system of algebraic equations in each cell of the mathematical model constrained by boundary conditions. The numerical solution strategy is depicted in Fig. 3.3 below.

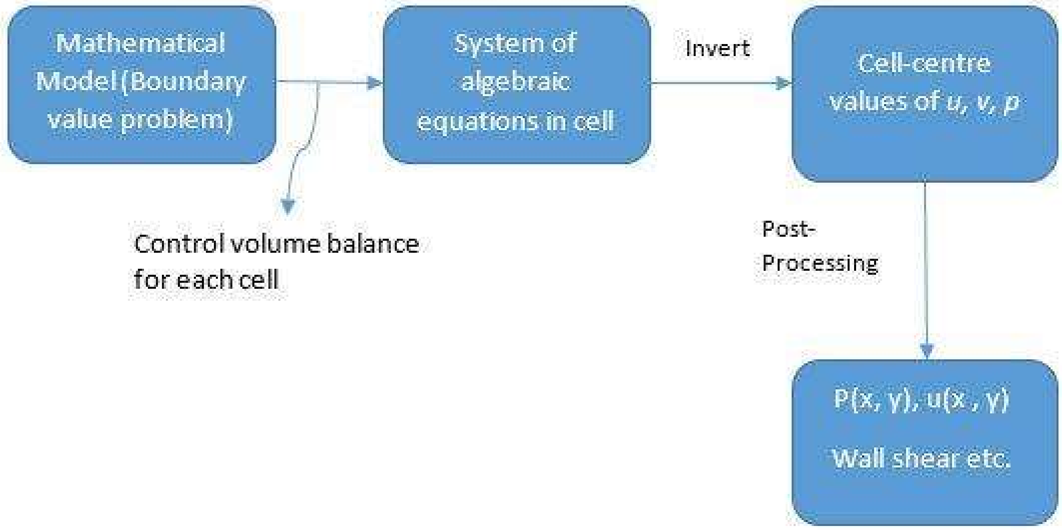

Figure 3. 3 Numerical solution strategy (Courtesy of A Hands-on Introduction to Engineering Simulations (edX) by Dr.Rajesh Bhaskaran)

3.6 Advantage of FVM Method Over Other Methods

An essential advantage of the finite volume method is that conservation is built into the method. The mass and momentum conservation equations are conserved in each cell.

FVM here differs from FEM in the methodology used to derive these systems of algebraic equations. In FEM control, volume balance is not performed in each cell. It is instead done by weighted integral form and using polynomial interpolations.

The Finite Difference Method (FDM) is also a differential form of the governing equations, where partial differential equations are directly converted to algebraic equations, but this method has one disadvantage: it cannot be easily extended to irregular meshes and complex domains. Most CFD problems like our present study involving flow around Piano key Weir involve complex domains and complex geometries. As such, in real engineering applications, FDM is seldom used in CFD codes. An overview of the discretization process followed in FVM and FEM is illustrated in Fig. 3.4 below.

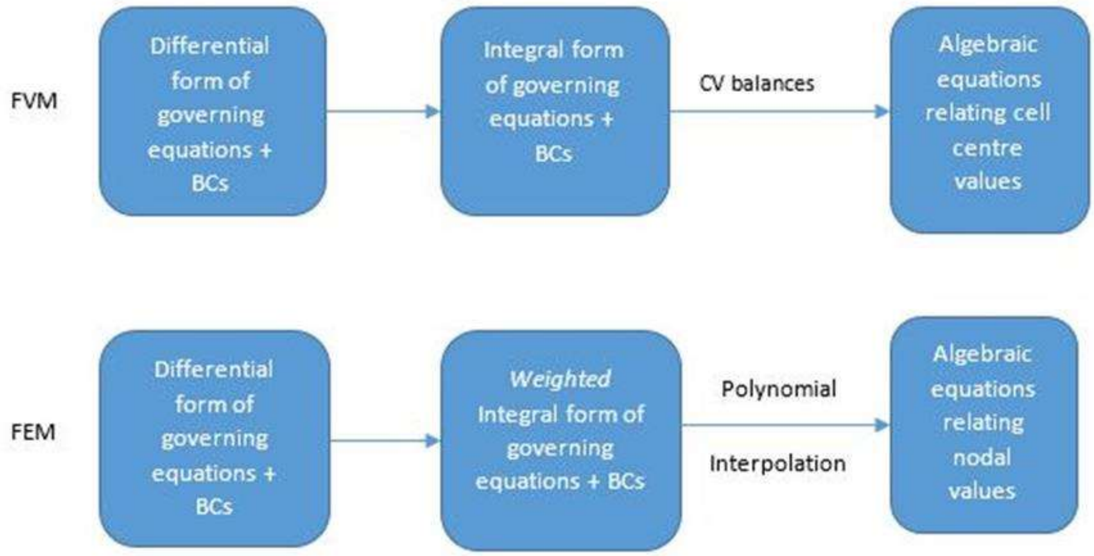

Figure 3. 4 FVM vs. FEM Models (Courtesy of A Hands-on Introduction to Engineering Simulations (edX) by Dr. Rajesh Bhaskaran).

3.7 Linearization Error and Deriving the System of Algebraic Equations

The system of algebraic equations derived by the FVM Method of control volume balancing has an additional complication. The additional complication refers to the algebraic equations being nonlinear.

As seen in the integral form of the momentum equation in Table 3.1, there is a nonlinear term. This nonlinear term is a product of two unknowns, i.e., the product of velocity times a velocity component. This set of nonlinear system of algebraic equations is solved by linearizing the nonlinear terms about some guess values, which introduces a new error called Linearization error. The CFD solver iterates the values around the guess values, updating the guess at each time. The iteration converges to give a good solution to the set of nonlinear systems of algebraic equations.

To decrease the linearization error, the CFD solver has to solve iteratively. The solver, after each iteration, updates the guess values until imbalances of mass and momentum are below some selected tolerance, and this linearization error becomes acceptable. Fig.

3.5 illustrates the iterative algorithm for the solution.

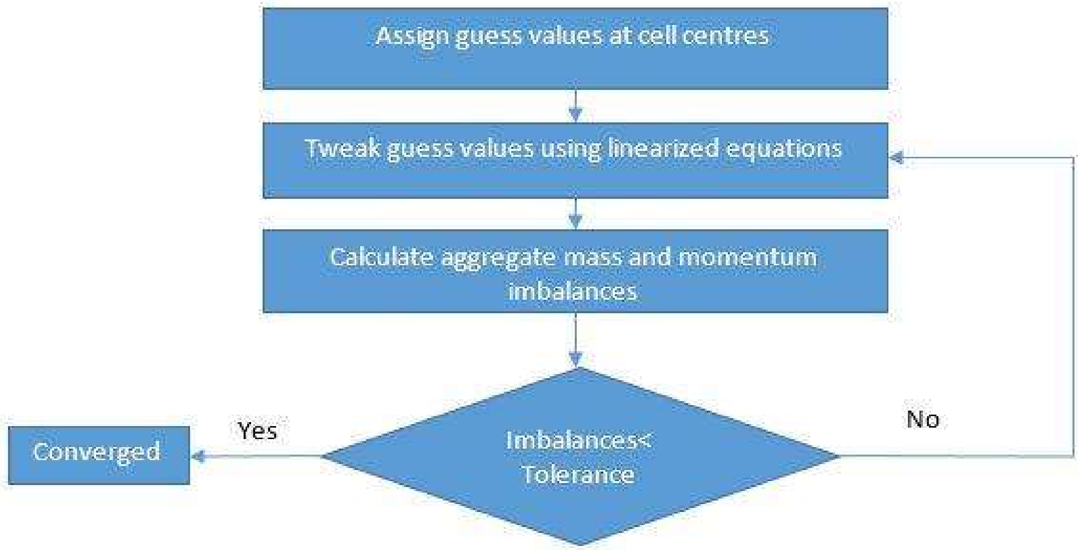

Figure 3. 5 Algorithm for iterative solution (Courtesy of A Hands-on Introduction to Engineering Simulations (edX) by Dr.Rajesh Bhaskaran)

Simply refining the mesh does not tend to decrease the overall error.

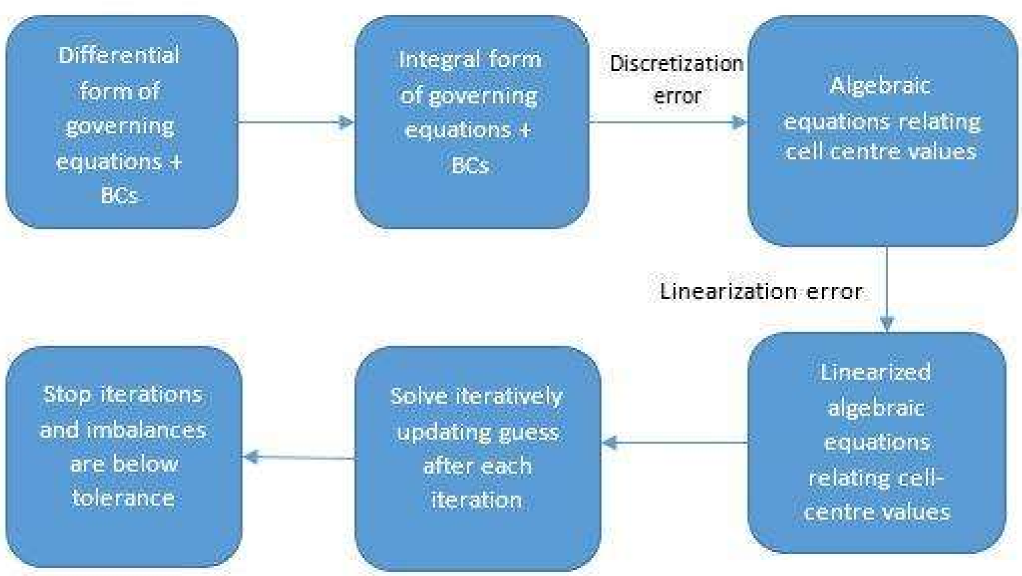

Figure 3. 6 Steps of numerical solution (Courtesy of A Hands-on Introduction to Engineering Simulations (edX) by Dr.Rajesh Bhaskaran)

The finer mesh makes the iterations harder to converge. Decreasing the discretization error makes the linearization error high, and as such, a balance between the two has to be maintained for getting an optimal solution through the CFD solver. The numerical solution steps are presented in Fig. 3.6.

3.8 Verification and Validation of the Numerical Study

Verification of the numerical model involves checking the mathematical model for numerical errors, comparison with hand calculations, mass and momentum imbalance check and as well as obvious trends as established by previous researchers.

Validation of the numerical model is checked by comparing the numerical results with experimental data.

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