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Comparison of the Coupled Solution of the Species, Mass, Momentum, and Energy Conservation Equations by Unstructured FVM, FDM, and FEM

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Abstract: In order to simulate fluid flow, heat transfer, and other related physical phenomena, it is necessary to describe the associated physics in mathematical terms. Nearly all the physical phenomena of interest to us in this book are governed by principles of conservation and are expressed in terms of partial differential equations expressing these principles. In this research paper, is a summary of conservation equations (Continuity, Momentum, Species, and Energy) that govern the flow of a Newtonian fluid. In particular, this paper studied the solution of two-dimensional (2D) Navier-Stokes (N-S) equations using the finite difference method (FDM), finite element method (FEM), and finite volume method (FVM) on a test problem of Methane combustion in a laminar diffusion flame. First, the computational domain was decomposed into grids in FDM and elements in FEM, later the Navier-Stokes equations, Energy, and, Species conservation equations were solved at the grid points and a MATLAB code has been written to check the consistency, stability, and accuracy for finer meshes. Following this step, the discretized equations for each sub-domain will be developed using the finite difference and finite element method, resolved using an iterative solver-Gauss Seidel technique. The MATLAB code is written for 2D geometries for science and engineering applications. The focus of this research paper is the development of physical models using numerical methods like FDM, and FEM for modeling science and Engineering applications by using Navier-stokes equations, Energy equations, and Species conservation equations.

Keywords: Coupled Solution, Conservation Equations, FDM, FEM, FVM

1. Introduction

Computational fluid dynamics (CFD) calculations of reacting flows or flows in which multiple species mix finds widespread use in a large number of practical applications. Examples include combustors, catalytic converters, and mixing devices in the chemical industry and in biological applications, among many others. In such calculations, mass conservation equations for individual species must be solved. The Navier-Stokes equation is a set of nonlinear partial differential equations describing the flow of fluids, representing the conservation of linear momentum. It is the cornerstone of fluid mechanics as noted by Cengel et al. [6]. It is solved jointly with the continuity equation. These equations cannot be solved exactly. So, approximations and simplifying assumptions are commonly made to allow the equations to be solved approximately. Recently, high-speed computers have been used to solve such equations by replacing them with a set of algebraic equations using a variety of numerical techniques like finite difference, finite volume, and finite element methods. The finite element method is the most powerful numerical technique for computational fluid dynamics which is readily applicable to domains of complex geometrical shape and provides great freedom in the choice of numerical

approximations. It reduces a partial differential equation system to a system of algebraic equations that can be solved using traditional linear algebra techniques. One of the major advantages of the finite element, finite difference, and finite volume method is that a general-purpose computer program can be developed easily to analyze various kinds of problems as noted by Kwon et al. [2]. In particular, a finite element method can easily handle any complex shape of a problem domain with prescribed boundary conditions Ghia et al. [4] studied high Reynolds number solutions for incompressible flow using the Navier-Stokes equation and the multigrid method. Persson [7] implemented a three-methods-based solver of the incompressible Navier-Stokes equations on unstructured two-dimensional triangular meshes. He solved the lid-driven cavity flow problem for four different Reynold numbers: 100, 500, 1000, and 2000. Gleisner et al. [11] discussed the three methods/ procedures for the Navier-Stokes equations in the primitive variable formulation and the vorticity stream function formulations. If the species interact with one another strongly, as in cases where chemical reactions or multi-component diffusion is present, it becomes numerically difficult to solve the species conservation equations in a sequential (or segregated) manner. These difficulties have been well-documented for reacting flow calculations. Recently, it has been demonstrated that a segregated solution is also prohibitive when the full multi-component diffusion equations are solved [9]. Sample calculations have shown that a simple problem involving g diffusive mixing of three species in a square box cannot be brought to convergence using a segregated solution approach even with strong under relaxation of the species Mazumder [12]. In this case too, as in cases with chemical reactions, the species are tightly coupled. In summary, in any problem in which the species are tightly coupled ugh the physics/chemistry mandates coupled solution of the species conservation equations. In general, coupled solution of a set of partial differential equations is the cornerstone for the simulation of a wide range of problems. Examples include e solution of Maxwell's equation [14] for electromagnetic phenomena, the radiative transfer equation [Mathur *et al.* [8], Mazumder [7] for heat transfer applications, and the Navier-Stokes equation Vanka [2], de Lemos [6] for fluid thermal-chemical phenomena, just to name a few. Thus, the volume of literature in this area is too large to have a comprehensive discussion in a limited space. Here, we will restrict ourselves to the discussion of pertinent methods and algorithms that have been prevalent for the simulation of fluid flow and associated phenomena, especially since the nature and technique for coupling the governing equations is, to a large degree, physics-dependent. Traditionally, in computational fluid dynamics (CFD), coupled solution of partial differential equations has their early roots in the aerospace area in which density-based time-marching methods are used. Compressing fluid flow results in a set of five (in three dimensions) coupled equations that are time-marched to a steady state using either explicit or implicit methods. Additional equations, such as the species conservation equations, are generally added as separate blocks and can be solved similarly. For example, Vanka [10] used this method for the implicit coupled solution of the Navier-Stokes equation in primitive variables. Duan *et al.* [6] have demonstrated this method for the solution of the coupled electric potential and species conservation equations in the context of fuel cell simulations, while Mazumder [9] has demonstrated it for the solution of the multi-component species diffusion equations. On an unstructured mesh, the discrete equations, when written in block-implicit form, result in a matrix that is sparse but not banded. Thus, line-by-line sweeps with block-tridiagonal inversion, as used for structured meshes, cannot be employed directly in this case. Nevertheless, the idea of using line-like sub-domains to perform line-by-line sweeps on unstructured meshes has been used successfully by Cete *et al.* Cete *et al*. [9] and by Li *et al.* Li *et al.* [9]—the so-called "unstructured ADI" method. It requires re-ordering of the cells and the compilation of additional connectivity information and is prohibitively tedious for three-dimensional (3D) computing-by-point-by-point block (or vector) Gauss-Seidel is a straightforward extension of the scalar Gauss-Seidel method for the solution of a coupled set of partial differential equations (PDE) on an unstructured mesh. However, as with scalar Gauss-Seidel, the spectral radius of convergence rapidly approaches unity as the mesh is refined, and the convergence deteriorates. Thus, the standalone block Gauss-Seidel is not attractive for large-scale computations of reacting flows. One approach to circumvent this problem is to use a multigrid method with block Gauss-Seidel as the smoother. In recent years, multigrid methods have become quite popular and are being widely used [Wesseling [4], Chow [2] Volker & Tobisca [15], Stüben [17], Walbroo [4], and Webster [10]. Of these, the algebraic multigrid (AMG) method Stüben [16], Walbro [14] has become the frontrunner on account of its ability to elegantly accommodate complex geometry and arbitrary unstructured mesh topology. In such methods, the linear algebraic equations are agglomerated (or added) to develop equations that philosophically correspond to equations for coarser geometric entities. The agglomeration strategy involves the comparison of link coefficients between adjacent cells. Research has now taken AMG methods for a single PDE (*i.e*., scalar case) to a level where the method has outshone most other methods because of its convergence characteristics and low memory requirements. In the case of coupled PDEs, however, issues remain. While the method has been used successfully for the solution of coupled PDEs Walbro [9], Raw [1], Webster [5], questions remain as to the best strategy for agglomerating two cells (or block algebraic equations) since each PDE now has a different set of link coefficients. In this work, a strategy that builds upon the "unstructured ADI" idea has been used. In the block Gauss-Seidel method, only variable-to-variable coupling is attained and all neighboring spatial cells are treated explicitly.

Marker and Cell (MAC) Method: This is an easy method to implement and involves the use of massless marker particles over the whole fluid domain [3]. A cell flagging procedure is

used over the domain, whereby a cell is either full, empty, or on a surface. A full cell initially is any cell with a marker particle present within it. An empty cell is any cell without a marker particle within it. A surface cell is any full cell adjacent to an empty cell. The MAC method can model highly deformed fluids and can also model detached and merging fluids. However, it is heavy on computer storage, especially in three dimensions, as every marker particle's position must be stored.

2. Objectives

2.1. General Objectives

The general objective of this research is to study the application of FDM and FEM on a Methane-Air combustion system in a laminar diffusive flame by solving the two-dimensional conservation equations numerically. To achieve this objective, efficient numerical methods are developed for a couple of solutions on momentum, energy, mass, and species conservation equations.

2.2. Specific Objectives

1) To analyze the stability, accuracy, convergence, and consistency of the FDM to solve the PDE numerically.
2) To analyze the stability, accuracy, convergence, and consistency of the FEM to solve the PDE numerically.
3) To study the nature of the mathematical model dictates the computational algorithms needed to solve the final set of governing equations for the three methods.
4) To write MATLAB programs for both analytical and numerical solutions.
5) Comparison of FDM & FEM using Navier-Stokes Equations for four conservation equations.

3. Governing Equations

Prior to the discussion of algorithms, it is necessary to discuss the governing equations and accompanying boundary conditions. Another motivation for a detailed discussion of the governing equations is that in low-speed reacting flow applications, which happen to be of interest to the authors, diffusive transport of mass is critical. Reacting flow formulations outlined in various textbooks and published articles pay little or no attention to diffusive (molecular) transport of species since turbulent transport dominates in the vast majority of applications of such flows. Thus, there is a need to critically assess commonly used formulations for the treatment of mass transport.

Continuity Equation:

$$\partial t + \nabla \cdot (\rho U) = 0$$

Momentum Equation:

$$\frac{\partial(\rho U)}{\partial t} + \nabla \cdot (\rho UU) = -\nabla P + \nabla \cdot \tau + \rho B$$

Energy Equation:

$$\frac{\partial(\rho_h)}{\partial t} + \nabla \cdot (\rho Uh) = -\nabla \cdot q + \dot{S_h}$$

Species Equation:

$$\frac{\partial(\rho Y_k)}{\partial t} + \nabla \cdot (\rho UYk) = -\nabla \cdot Jk + \dot{S_k}$$

where ρ is the mixture density, p is the pressure, τ is the shear stress tensor, and B the body force vector. The continuity equations and Momentum equations are the well-known Navier–Stokes equations and need no further discussion. In the Species equation, Y_k is the mass fraction of the kth species, J_k is the mass diffusion flux of the kth species, and $\dot{S_k}$ is the production rate of the kth species due to homogeneous chemical reactions. The total number of gas-phase species in the system is denoted by N. In the energy equation, $\dot{S_h}$ represents the net source due to viscous dissipation and other work and heat interactions, and q denotes the net heat flux due to molecular conduction, radiation, and inter-species diffusion.

4. Test Problem

Combustion is one of the most important processes in engineering, which involves turbulent fluid flow, heat transfer, chemical reaction, radiative heat transfer, and other complicated physical & chemical processes. Typical engineering applications include internal combustion engines, power station combustors, aero engines, gas turbine combustors, boilers, furnaces, and much other combustion equipment. It is important to be able to predict the flow, temperatures, resulting species concentrations, and emissions from various combustion systems for the design and improvement of combustion equipment, particularly with the current concerns about CO_2 and other emission levels and their effects on the environment. CFD lends itself very well to the modeling of combustion. Combustion processes are governed by basic transport equations for fluid flow and heat transfer with additional models for combustion chemistry, radiative heat transfer, and other important sub-processes. There are many types of combustion processes. Gaseous fuel combustion, liquid fuel combustion, spray combustion, solid fuel combustion, and pulverized fuel combustion are a few of the many other processes used in a wide variety of application areas. To illustrate the application of CFD we concentrate on gaseous combustion. For other processes the relevant literature to find out how CFD has been successfully applied in areas like spray combustion (Beck and Watkins, 200pulverizedised coal combustion (Lockwood *et al*., [9], diesel and spark ignition engines (Blunsdon *et al*., 1992, 1993; Henson and Malalasekera, [6] a modeling tool. Gaseous combustion involves a chemical reaction between a fuel and an oxidant that are both in the gas phase.

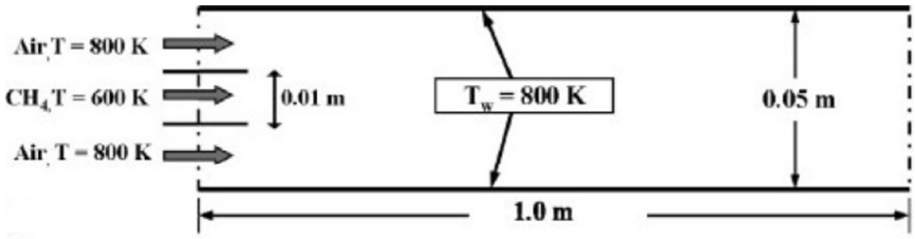

Figure 1. *2D Geometry where the methane-air mixture is combusted.*

There are two categories of gaseous combustion processes: premixed combustion and non-premixed combustion. For example, combustion in a spark ignition internal combustion engine (petrol engine) can be categorized as premixed combustion, as the fuel (gasoline) is mixed with air prior to combustion, which takes place after spark ignition. Similarly, the flame in the familiar Bunsen burner is also premixed combustion, as air is allowed to mix with gas prior to combustion. By contrast, a jet flame where the fuel enters ambient air and is allowed to burn is an example of a non-premixed flame. The gaseous fuel mixes with the oxidant stream (air) and then combustion takes place where the conditions are right.

In addition, we conclude the above test problem s follows:

1) The test problem considered for the present study is that of a homogeneous combustion methane-airline–air mixture under laminar flow conditions, that is, a laminar flame.
2) A simple two-dimensional (2D) diffusion flame configuration, as shown in Figure 1, is considered. Based on the inlet conditions, the overall equivalence ratio is unity, and the Reynolds number based on the channel width is approximately 150.
3) A 2-step reaction mechanism involving 6 gas-phase species (CH_4, CO_2, H_2O, N_2, O_2, CO) was used for gas-phase chemistry calculations.

5. Discretization with FEM and FDM

Before discretizing with numerical methods, it is to be noted that to make the conservation equations simpler all the conditions of the system must be defined. Known conditions are:

i. Reynolds No.: 150 approximately
ii. X domain length: 1m
iii. Y domain length: 0.05m
iv. Wall Temperature: 800K
v. Inlet Air Temperature: 800K
vi. Inlet Methane Temperature: 600K
vii. Equivalence Ratio: 1
viii. FDM via MAC algorithm

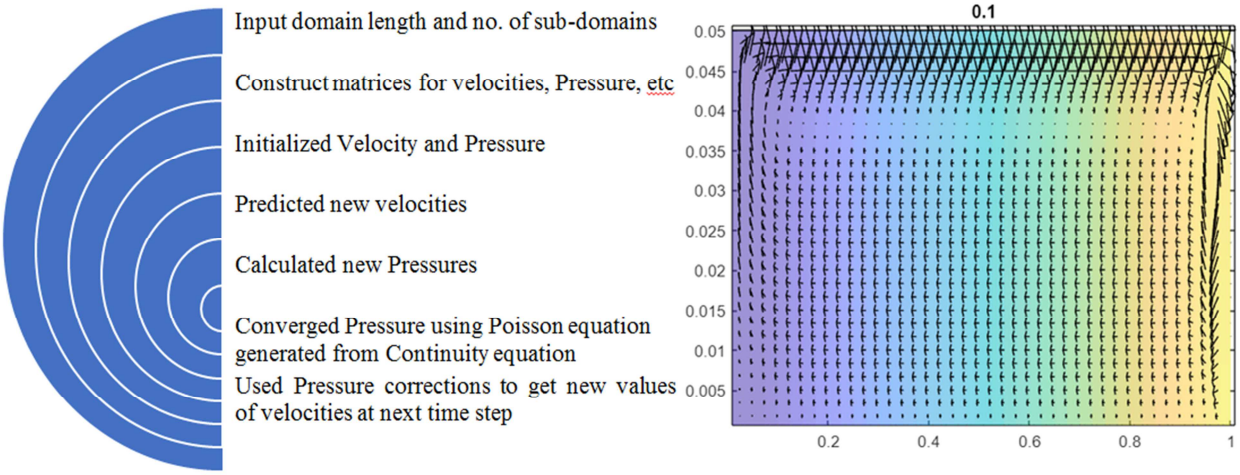

Figure 2. *FDM via MAC algorithm.*

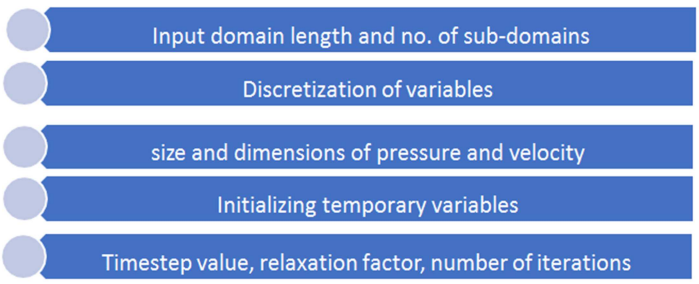

Figure 3. *Initializing temporary variables.*

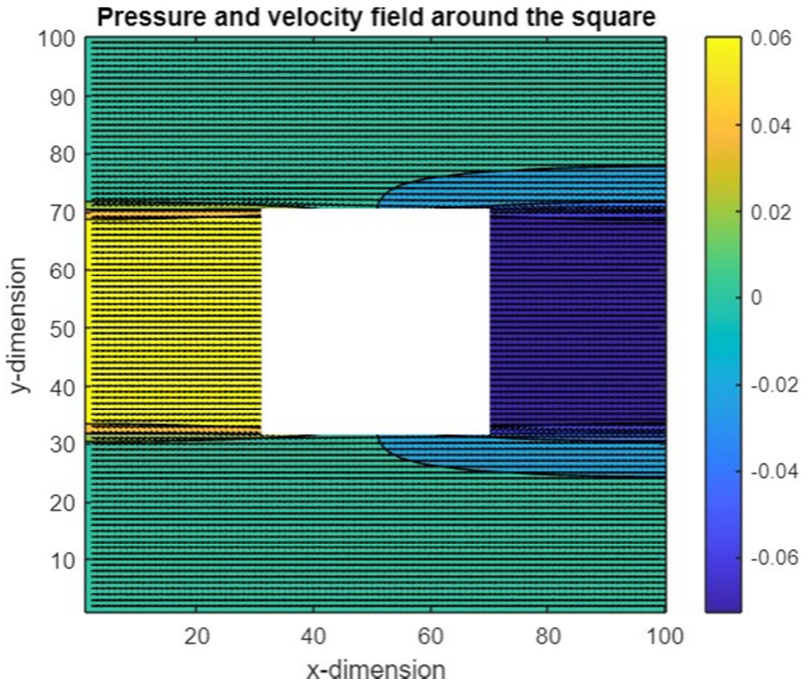

Figure 4. *FEM via Galerkin method.*

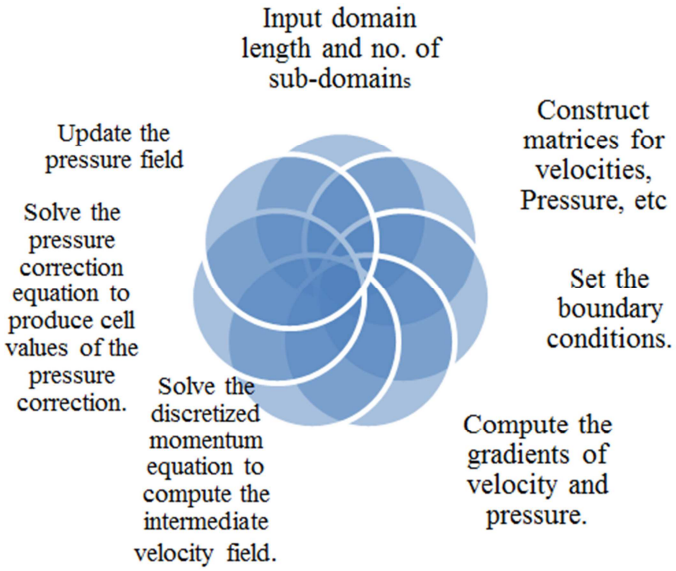

Figure 5. *FVM via* a *SIMPLE algorithm.*

6. Conclusions

To illustrate the finite difference and finite element method discussed in this project we considered a square lid-driven cavity flow of length 1 unit and breadth 0.05 unit. The boundary conditions are such that the flow is driven by a unit horizontal velocity at the top boundary. In this project work, we discussed finite difference via the Marker and Cell method abbreviated as MAC as well as finite element via the Galerkin Finite element method solution of the two-dimensional structured or incompressible Navier-Stokes equation, species and energy equations by the benchmark of the square lid-driven cavity and compared it with 2D structured FVM via SIMPLE algorithm. Dirichlet boundary conditions were imposed on every boundary of the domain. The finite element programming codes were constructed to solve these equations. Having studied some of the basic features and difficulties with simulating incompressible fluid flow we now turn to consider the full-fledged Navier-Stokes equations and proceed to solve the Energy and Species equations which in addition to the Stokes system are both non-linear and time-dependent. Indeed, the Navier-Stokes equations, species, and energy conservation equations are so complex that their numerical study has grown into a discipline of its own called computational fluid dynamics, abbreviated CFD. These project work programming codes are written using MATLAB R2021b.

References

[1] Coupled solution of the species conservation equations using the unstructured finite-volume method: Ankan Kumar and Sandip Mazumder, 2009.

[2] Mazumder S. Critical assessment of the stability and convergence of the equations of multi-component diffusion. Journal of Computational Physics 2006; 212 (2): 383–392.

[3] Kuo KK. Principles of Combustion. Wiley: New York, 1986.

[4] Bird RB, Stewart WE, Lightfoot EN. Transport Phenomena (2nd ed). Wiley: New York, 2001.

[5] Toselli A, Widlund O. Domain Decomposition Methods — Algorithms and Theory. Springer Series in Computational Mathematics, vol. 34. Springer: New York, 2004.

[6] Sung K, Shirley P. Ray tracing with a BSP tree. In Computer Graphics Gems III, Kirk D (ed.). AP Professional: San Diego, CA, 1992; 271–274.

[7] Karypis G, Kumar V. A fast and high-quality multilevel scheme for partitioning irregular graphs. SIAM Journal on Scientific Computing 1998; 20: 359–392.

[8] Henk Kaarle Versteeg, Weeratunge Malalasekera, *An Introduction to Computational Fluid Dynamics: The Finite Volume Method*, Pearson Education Limited, 2007.

[9] Petrila, Titus, Trif, Damian, Basics of Fluid Mechanics and Introduction to Computational Fluid Dynamics, Springer Publication, 2012.

[10] Hassan Khawaja (2021). SIMPLE (https://www.mathworks.com/matlabcentral/fileexchange/66129-simple), MATLAB Central File Exchange. Retrieved November 29, 2021.

[11] R Surya Narayan (2022). Navier-Stokes Solver using SIMPLE (https://www.mathworks.com/matlabcentral/fileexchange/74996-navier-stokes-solver-using-simple), MATLAB Central File Exchange. Retrieved October 19, 2022.

[12] B. R. Baliga and S. V. Patankar. A control-volume finite element method for two-dimensional fluid flow and heat transfer. Numerical Heat Transfer, 6: 245–261, 1983.

[13] C. Hsu. A Curvilinear-Coordinate Method for Momentum, Heat and Mass Transfer in Domains of Irregular Geometry. Ph.D. thesis, University of Minnesota, 1981.

[14] C. M. Rhie and W. L. Chow. A numerical study of the turbulent flow past an isolated airfoil with trailing edge separation. AIAA Journal, 21: 1525–1532, 1983.

[15] M. Peric. A Finite Volume Method for the Prediction of Three-Dimensional Fluid Flow in Complex Ducts. Ph.D. thesis, University of London, August 1985.

[16] S. Majumdar. Role of under relaxation in momentum interpolation for calculation of flow with non-staggered grids. Numerical Heat Transfer, 13: 125–132, 1988.

[17] J. Y. Murthy and S. R. Mathur. Computation of anisotropic conduction using unstructured meshes. Journal of Heat Transfer, 120: 583–591, August 1998.