UNIVERSITAT POLITÈCNICA DE CATALUNYA

BACHELOR'S DEGREE IN AEROSPACE
TECHONOLOGIES ENGINEERING

BACHELOR'S THESIS - REPORT

Study of the computational resolution of conservation equations of mass, momentum and energy in different aeronautical and industrial engineering problems

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1 Introduction

1.1 Aim

Study for the computational resolution of conservation equations of mass, momentum and energy in fluid-body problems. The main goal of the project is to determine the changes ocurred in a fluid when contacting with a solid body using different methods, laws and solvers.

1.2 Scope

The main objectives to achieve are:

- Study of the potential flow in a channel and around a solid object such as a cylinder or a NACA airfoil.

- Study of the variation in temperature, pressure, velocity and density in a parallel flux in a channel or around a cylinder.

- Solving the system of equations using different solver methods: Gauss-Seidel, line-by-line, TDMA...

- Solving Navier Stokes equations using methods: implicit, explicit, Crank-Nicholson...

- Study of the Conduction-Difussion equation for different problems: case in which the velocity field is known, transient case...

- Study of the turbulence using different methods: DNS, LES and RANS in a plate and around a cylinder

- Comparison when possible between the results obtained using the developed software and the results obtained by analythical means

- Redaction of the report in which there will be a theorical explanation of the equations, and the results obtained.

- Programming the solving codes in lenguage C++ using the platform *Visual Studio Code*. For the plots and graphs, $MATLAB^{®}$ will be used.

- Study of the computational costs of the codes developed during the realization of the project

1.3 Requirements

The requeriments of the Bachelor's Thesis are the following:

- The Project dedication limit is 300 hours (12 ECTS).

- All academic documents will be written in English.

- The deadline of the Project is June 10th, 2019.

- The presentation of the Project will be held between July 8th and July 19th.

- All the programs have to be developed in lenguage C++ without using any kind of simplying solvers or software developed by another user.

- For plotting graphs (heat maps, vector fields, y-x graphs, isotherms, streamlines...) MATLAB® will be used. MATLAB® will be only used to represent the data obtained in a graph, another post-process program can be used.

1.4 Justification

1.5 Background

Nowadays, there are plenty of programs and software able to solve Navier Stokes equations and turbulence. Some of them are open source programs (*OpenFoam*) while others are mainly commercial (*Autodesk CFD*, *Fluent* in Ansys or the Toolbox *CFDTool* in MAT-LAB).

These software is used by companies, at University or even at user level. They are capable of solving the interaction between a fluid with a solid, and determine parameters like temperature, velocity, pressure, density, heat, energy... These software are given the name of CFD (Computational Fluid Dynamics).

The huge evolution in computers ocurred in the last 10 years, especially in the CPU (Central Processing Unit) and of course to the RAM memories (Random Access Memory), has increased the speed and potencial of calculus that years before where hardly impossible to imagine.

Simulations offer estimations and allow us to analize big complex problems for which there is no analythical solution yet. Once a model is determined, inserting the code with the actions in the computer, results can be achieved.

Nevertheless, the main inconvenience is that sometimes the most suitable way to solve a given equation leads to a huge amount of computational time and money that the user cannot afford. Although, with new technologies arrivals and developments these aspects will be diminished in the years yet to come.

On the other hand, the main problem that the software has to solve is the turbulence. Turbulence can be defined as any pattern of fluid motion characterized by chaotic changes in pressure and flow velocity. Most of the software mentioned before uses turbulence resolution methods. The most popular ones are:

- DNS (Direct Numerical Solution)

- RANS (Reynolds Average Numerical Solution)

- LES (Large eddy simulation)

The idea of the Project is to explain and understand the main ideas of the Physical, Thermodynamical, Aerodynamical principles between the commonly used by this software and being able to solve some fluid-body problems of less complexity.

2 Numerical Analysis

3   Potential Flow

On this chapter, there will be developed the potential flow solution in a duct of constant section and also around a cylinder and a NACA airfoil using different solvers.

The flow region around aerodynamic bodies can be divided into:

- **Boundary Layer region**. Area closed to the walls of the body with a small thickness. High gradient of pressure and temperature are produced within, due to the friction, heat transfer and mainly turbulence.

- **Inviscid region**. Rest of the domain in which the effects of friction and heat losses can be neglected.

The Inviscid region is governed by Euler's equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \qquad (Conservation\ of\ Mass) \tag{3.1}$$

$$\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p \qquad (Conservation\ of\ Momentum) \tag{3.2}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot (E \vec{v}) = -\nabla \cdot (p \vec{v}) \qquad (Conservation\ of\ Energy) \tag{3.3}$$

where E represents the total energy (kinetic + internal) per unit of volume.

The external flows around bodies can be considered as inviscid (frictionless) and irrotational (the fluid particles are not rotating). Therefore, the viscous effects are limited to a thin layer next to the body called the boundary layer.

3.1   Potential function

A potential function ϕ(x,z,t) can be defined as a continuous function that satisfies the conservation of mass and momentum, assuming incompressible, inviscid and irrotational flow.

For a scalar function ϕ the following equation, while by definition for the irrotational flow:

$$\nabla \times \nabla \phi = 0 \qquad (3.4) \qquad\qquad \nabla \times \vec{v} = 0 \qquad (3.5)$$

Thereofe, a velocity potential function ϕ(x,y,z,t) can be obtained:

$$\vec{v} = \nabla \phi \tag{3.6}$$

The components of velocity in Cartesian coordinates are:

$$u = \frac{d\phi}{dx} \qquad\qquad v = \frac{d\phi}{dy} \qquad\qquad w = \frac{d\phi}{dz}$$

The velocity field must satisfy the conservation of mass equation. Replacing the each term, and introducing the definition of the velocity components:

$$\rho(\frac{\partial u}{dx} + \frac{\partial v}{dy} + \frac{\partial w}{dz}) = 0 \; \rightarrow \; \frac{\partial^2(\phi)}{dx^2} + \frac{\partial^2(\phi)}{dy^2} + \frac{\partial^2(\phi)}{dz^2} = 0 \qquad (3.7)$$

The Laplace equation is obtained:
$$\nabla^2 \phi = 0 \qquad (3.8)$$

The Laplace equation can be solved in different coordinate systems: cartesian, cylindrical or spherical (see in [1]).

Lines of constant ϕ are called potential lines. In two dimensions:

$$d\phi = \frac{\partial(\phi)}{\partial x} dx + \frac{\partial(\phi)}{\partial y} dy \; \rightarrow \; d\phi = u dx + v dy \qquad (3.9)$$

Since $d\phi = 0$ along a potential line:

$$\frac{dy}{dx} = -\frac{u}{v} \qquad (3.10)$$

Recall that streamlines are lines tangent to the velocity; $\frac{dy}{dx} = \frac{u}{v}$. Streamlines are perpendicular to the potential lines and a scalar function to streamlines can be described too, named as Stream Function Ψ. The relations between each are:
$$u = \frac{\partial \phi}{\partial x} = \frac{\partial \Psi}{\partial y} \qquad\qquad v = \frac{\partial \phi}{\partial y} = -\frac{\partial \Psi}{\partial x}$$

These equations are also known as the Cauchy-Riemann equations.

3.2 Stream Function

For a 2D potential flow, assuming incompressible, inviscid and irrotational flow a Stream Function can be determined [2]. The velocities expressed as a function of the stream function are:

$$v_x = \frac{\rho_0}{\rho} \frac{d\Psi}{dY} \qquad (3.11) \qquad v_y = -\frac{\rho_0}{\rho} \frac{d\Psi}{dX} \qquad (3.12)$$

where ρ_0 is the reference density for determined conditions (p_o, T_0).

Obviously, the stream function verifies the conservation of mass equation ($\nabla \cdot (p\vec{v} = 0)$. While the vorticity is defined as:

$$\vec{\omega} = \nabla x \vec{v}$$

Subtituting, it is obtained:

$$\frac{\partial}{\partial x}\left(\frac{\rho_0}{\rho}\frac{d\Psi}{dx}\right) + \frac{\partial}{\partial y}\left(\frac{\rho_0}{\rho}\frac{d\Psi}{dy}\right) = -\omega_z$$

Given that the flow is considered irrotational ($\omega_z = 0$).

$$\frac{\partial}{\partial x}\left(\frac{\rho_0}{\rho}\frac{d\Psi}{dx}\right) + \frac{\partial}{\partial y}\left(\frac{\rho_0}{\rho}\frac{d\Psi}{dy}\right) = 0$$
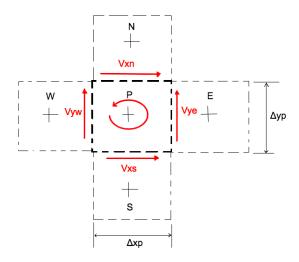

Figure 3.1: Circulation in an intern CV

The ciculation in an intern Control Volume (CV), such as the one in Figure 3.1 is:

$$\Gamma = v_{ye}\,\triangle\,y_P - v_{xn}\,\triangle\,x_p - v_{yw}\,\triangle\,y_p + v_{xs}\,\triangle\,x_p = 0 \tag{3.13}$$

The velocities in the faces of the Control Volume (CV) are obtained:

$$V_{ye} = -\frac{\rho_0}{\rho_e}\frac{d\Psi}{dx}\bigg|_e \approx \frac{-\rho_0}{\rho_e}\frac{\Psi_E - \Psi_P}{d_{PE}} \qquad V_{yw} = \frac{\rho_0}{\rho_w}\frac{d\Psi}{dx}\bigg|_w \approx \frac{\rho_0}{\rho_w}\frac{\Psi_W - \Psi_P}{d_{PW}}$$

$$V_{xn} = \frac{\rho_0}{\rho_n}\frac{d\Psi}{dy}\bigg|_n \approx \frac{\rho_0}{\rho_n}\frac{\Psi_N - \Psi_P}{d_{PN}} \qquad V_{xs} = -\frac{\rho_0}{\rho_s}\frac{d\Psi}{dy}\bigg|_s \approx \frac{-\rho_0}{\rho_s}\frac{\Psi_S - \Psi_P}{d_{PS}}$$

Introducing the definition of velocities in the Eq. 3.13.

$$-\frac{\rho_0}{\rho_e}\frac{\Psi_E - \Psi_P}{d_{PE}}\,\triangle\,y_p - \frac{\rho_0}{\rho_n}\frac{\Psi_N - \Psi_P}{d_{PN}}\,\triangle\,x_p + \frac{\rho_0}{\rho_w}\frac{\Psi_P - \Psi_W}{d_{PW}}\,\triangle\,y_p + \frac{\rho_0}{\rho_s}\frac{\Psi_P - \Psi_S}{d_{PS}}\,\triangle\,y_s = 0$$

Finally, the equation of discretization is:

$$a_P\Psi_P = a_E\Psi_E + a_W\Psi_W + a_N\Psi_N + a_S\Psi_S + b_P$$

where each term corresponds to:

$$a_E = \frac{\rho_0}{\rho_e}\frac{\triangle y_p}{d_{PE}}; \qquad a_W = \frac{\rho_0}{\rho_W}\frac{\triangle y_p}{d_{PW}}; \qquad a_N = \frac{\rho_0}{\rho_N}\frac{\triangle y_p}{d_{PN}};$$

$$a_S = \frac{\rho_0}{\rho_S}\frac{\triangle y_p}{d_{PS}}; \qquad a_P = a_E + a_W + a_N + a_S; \qquad b_P = 0$$

3.2.1 Parallel flow in a duct

A constant and parallel flow ($u_x = u$, $v_y = 0$) is moving towards a duct of constant section. Integrating Eq. 3.11 and Eq. 3.12, the stream function Ψ has the following expresion (Eq. 3.14):

$$\Psi = \frac{\rho_0}{\rho}u_x \cdot Y + \frac{\rho_0}{\rho}v_y \cdot X + k \tag{3.14}$$

In this case, the velocity in y-direction is null and the value of the constant k is imposed as 0. The following equation is obtained:

$$\Psi = \frac{\rho_0}{\rho}u \cdot Y \tag{3.15}$$

The analythical solution correspond to lines parallel to the x-axis, that increase their value has Y increases.

A program to solve the problem has been developed *ParallelFlow.cpp* (Code in *Annex 1*). With the graphic library of *MATLAB*®, the streamlines of the solution has been represented in Figure 3.3.

The problem has been solved using Gauss-Seidel, which is a point by point solver and in every loop the convergence of the solution is checked ($|\phi_{new}[i] - \phi[i]| > \delta$). If the answer is true, then $\phi[i] = \phi_{new}[i]$, if not $\phi[i]$ remains with the same value.

In this case, for the solver ther have been implemented two different solvers: Gauss-Seidel and TDMA line-by-line. These solvers are explained in the following sections.

3.2.1.1 Gauss Seidel

Gauss-Seidel is an iterative method used to solve a linear system of equations, it is a point-by-point solver. For example, for the case *Parallel flow in a duct* the equation to solve has the following structure [3].

$$a_p \cdot \phi_p = a_e \cdot \phi_e + a_w \cdot \phi_w + a_n \cdot \phi_n + a_s \cdot \phi_s + b_p$$

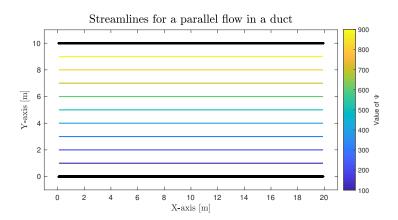Therefore, for the calculation of ϕ at the node P (ϕ_p):

Figure 3.2: Streamlines of a parallel flow in a duct

Figure 3.3: Resolution's diagram of Parallel Flow problem

$$\phi_p = \frac{a_e \cdot \phi_e + a_w \cdot \phi_w + a_n \cdot \phi_n + a_s \cdot \phi_s + b_p}{a_p}$$

The value of ϕ in the domain is calculated in every point, taking into account the values of the nodes nearby.

3.2.1.2 TMDA : Line-by-line

Line-by-line is a TDMA solver (Tridiagonal matrix algorithm) which is only valid for matrix where its main diagonal, and upper and lower are different from zero, the rest of terms are null or almost zero.

This solver is capable of solving equations with the following structure:

$$a_p \cdot \phi_p = a_e \cdot \phi_e + a_w \cdot \phi_w + b_p$$

However, for 2D cases it is possible to transform the equation into (line-by-line method):

$$a_p \cdot \phi_p = a_e \cdot \phi_e + a_w \cdot \phi_w + b_p^*$$

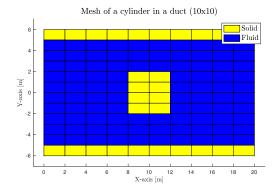where: $b_p^* = a_n \cdot \phi_n + a_s \cdot \phi_s + b_p$

TDMA method is quicker than Gauss-Seidel method. For several cases TDMA does not need a convergence criterion, so it is a direct method, whereas Gauss-Seidel method is an iterative method so a loop is needed to achieve the convergence.

3.2.2 Flow around a cylinder

In this case, the mesh has to be determined carefully. It has to be taking into account that a part of the mesh would be solid and the other, fluid. The *Blocking Off* method has been implemented to solve determine the nodes of fluid and the ones of solid.

The *Blocking Off* method evaluates if the centroid of the Control Volume (CV) is either in the fluid domain or in the solid domain. The higher density the mesh is, the more accurate the discretization will be.

In Figure 3.4 the mesh has a dimension of 10x10 ((Nx)x(Ny), where, Nx and Ny are the number of divisions along the x-axis and y-axis), it is easy to observe that the shape of the cylinder is not well defined. Whereas, in Fig. 3.5 and Fig. 3.6, for the meshes of size 50x50 and 100x100 respectively, the definition has improved.
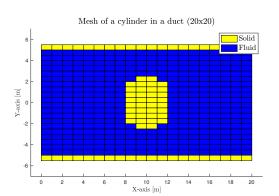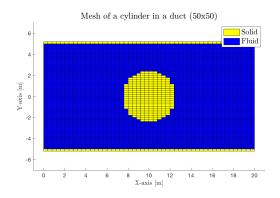

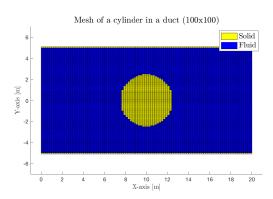Figure 3.4: BOM - Cylinder with a mesh of dimensions 10x10

Figure 3.5: BOM - Cylinder with a mesh of dimensions 20x20

Figure 3.6: BOM - Cylinder with a mesh of dimensions 50x50

Figure 3.7: BOM - Cylinder with a mesh of dimensions 100x100

In this case, the dimensions of the problem are:

- Lenght of the duct : L = 20 m

- Height of the duct : H = 10 m

- Radius of the cylinder : R = 2.5 m

And the velocidy field at the entrance is known:

- $u_x = u_{inf} = 50\frac{m}{s}$

- $v_x = 0$

The Mach number for the entrance velocity is $M = {}^v/_{v_{sound}} = \frac{50m/s}{340m/s} = 0.147$. Therefore, the flow can be considered incompressible (M<0.2).

The cylinder is centered in the middle of the channel. A program to solve the problem has been developed *phiCylinder.cpp* (Code in *Annex 1*). In Figure 3.8, the solution of the streamlines around a cylinder can be observed.

The boundary conditions established were the following:

- The velocity in the entrance has a constant value ($u_x = u_{inf}$ and $v_x = 0$). Therefore, stream function Ψ is also known, substituting in the Eq.3.14.

- The stream function Ψ on the walls is known ($u_x = u_{inf}$ and $v_x = 0$). There is no normal velocity in the nodes in the wall, only tangential velocities.

- The shape of the cylinder corresponds to a stream line its self and it is a constant value.

An analythical solution [4] to the flow around a cylinder (Eq. 3.16) can be obtained. The solution is the superposition the stream function of a uniform flux and a dipole.

$$\Psi = \Psi_U + \Psi_D = V_\infty r sen(\theta)(1 - \frac{R^2}{r^2}) \tag{3.16}$$
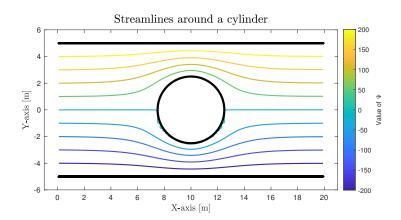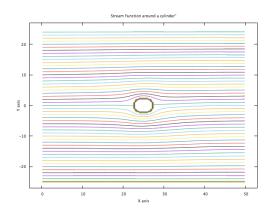
13

Figure 3.8: Streamlines around a cylinder

The next step would be to compare the obtained solution with the analytical. Because of the effect of the walls and their boundary conditions, there is a considerable difference between them, due to the fact that analythical solution doesn't take the walls into account.

In order to compare the solution obtained with the analytical solution correctly, there are two possibilities:

- Increase the distance between the cylinder and the walls of the channel, in order to reduce the interference.

- Establish new boundary conditions. The new boundary conditions will correspond to the analytical stream function obtained at the points of the wall.

In the first possibility, the maximmum error obtained in a point is 3.15%. In Figure 3.9 and Figure 3.10 the analytical and the solution obtained with the program can be observed. A program to compare both solutions has been developed *CylinderError1.cpp* (Code in *Annex 1*).

While, for the second possibility the maximmum error obtained in a point is 0%. Therefore, it can be established that the program solves perfectly the problem. In Figure 3.11 and Figure 3.12, both the solutions can be observed. A program to compare both solutions has been developed *CylinderError2.cpp* (Code in *Annex 1*).
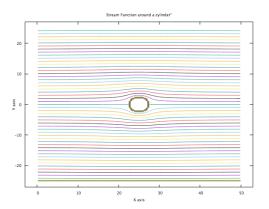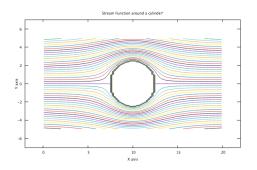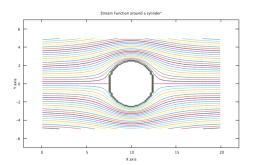
Figure 3.9: Stream Function Solution obtained with the solver - Case 1

Figure 3.10: Analytical stream function solution - Case 1

Figure 3.11: Stream Function Solution obtained with the solver - Case 2

Figure 3.12: Analytical stream function solution - Case 2

3.2.3 Flow around a NACA airfoil

As done with the cylinder, Blocking Off method is used to determine the mesh and its boundary conditions. In this case of a NACA airfoil is placed in the middle of the duct (Figure 4.2 and Figure 4.3).

The dimensions of the problem were:

- Lenght of the duct : L = 20 m
- Height of the duct : H = 10 m

And for the chracterisitics of the airfoil:

- Chord : c = 9 m
- Thickness : t = 1.5 m
- Angle of attack : $\alpha = 10^o$

And the velocidy field (incompressible case) at the entrance is known:
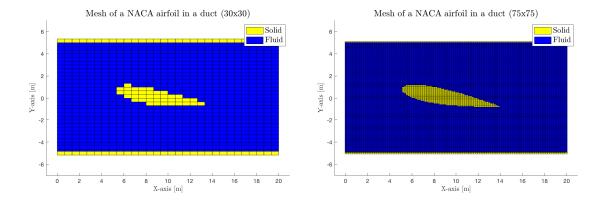
Figure 3.13: BOM - NACA profile with a mesh of dimensions 30x30

Figure 3.14: BOM - NACA profile with a mesh of dimensions 75x75

- $u_x = u_{inf} = 50\frac{m}{s}$

- $v_x = 0$

A program to solve the problem has been developed *NACAsolution.cpp* (Code in *Annex 1*). In Figure 3.15, the streamlines around a NACA airfoil can be observed. In this case the solution obtained has been obtained under the hyphothesis of potential flow and incompressible, therfore the flow around the NACA airfoil, and the cylinder solved in the previous sections, is attached.
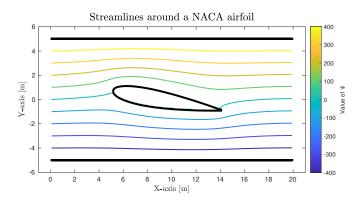
Figure 3.15: Streamlines around a NACA airfoil

3.3 Potential Flow resolution

In order to solve Potential flow problems the sequence of actions and calculations are resumed in Figure 3.16.

3.4 Summary

Figure 3.16: Diagram of the resolution of Potential Flow problem

4 Convection-diffusion

On this chapter, there will be developed a solution of the Convection-diffusion equation of the momentum equation for the case in which the velocity field is known.

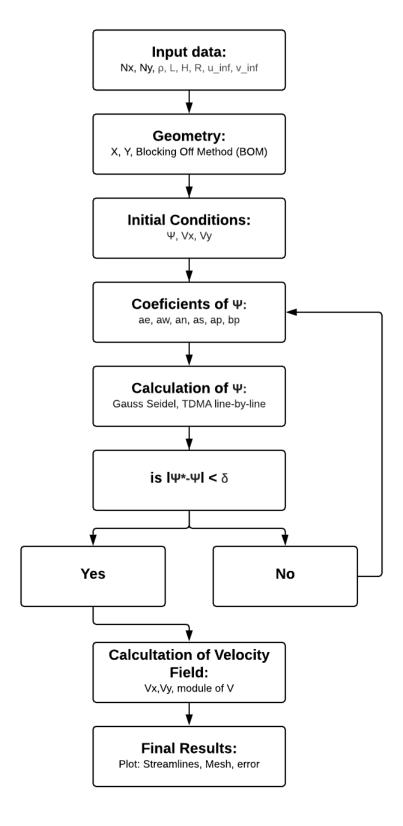## 4.1 Convection-diffusion equation

Navier-Stokes equations for perfect gases ($c_v = $ constant) can be written as:

$$\underbrace{\frac{\partial \rho}{\partial t}}_{unsteady\ term} + \underbrace{\nabla \cdot (\rho \vec{v})}_{convective\ term} = 0 \tag{4.1}$$

$$\underbrace{\frac{\partial (\rho \vec{v})}{\partial t}}_{unsteady\ term} + \underbrace{\nabla \cdot (\rho \vec{v} \vec{v})}_{convective\ term} = - \underbrace{\nabla \cdot (\mu \nabla \vec{v})}_{diffusion\ term} + \{\nabla \cdot (\vec{\tau} - \mu \nabla \vec{v}) - \nabla p + \rho \vec{g}\} \tag{4.2}$$

$$\underbrace{\frac{\partial (\rho T)}{\partial t}}_{unsteady\ term} + \underbrace{\nabla \cdot (\rho \vec{v} T)}_{convective\ term} = \underbrace{\nabla \cdot (\frac{\lambda}{c_v} \nabla T)}_{diffusion\ term} + \{\frac{-\nabla \cdot \vec{q}^R - \nabla p \cdot \vec{v} + \vec{\tau} : \nabla \vec{v}}{c_v}\} \tag{4.3}$$

These equations are formed by a unsteady term (which depends on time), a convective term, a diffusive term can be found and other terms [5].

Equation	ϕ	Γ_ϕ	s_ϕ
Mass	1	0	0
Momentum	$\vec{v}$	μ	$\nabla \cdot (\vec{\tau} - \mu \nabla \vec{v}) - \nabla p + \rho \vec{g}$
Energy	T	λ/c_v	$(-\nabla \cdot \vec{q}^R - \nabla p \cdot \vec{v} + \vec{\tau} : \nabla \vec{v})/c_v$

Table 4.1: Navier-Stokes equations into convection diffusion transport form

Therefore a generic variable ϕ (e.g. velocity, temperature, mass, entropy, etc.) the equations can be written into a generic convection diffusion transport equation [6]:

$$\frac{\partial (\rho \phi)}{\partial t} + \nabla \cdot (\rho \vec{v} \phi) = \nabla \cdot (\Gamma_\phi \nabla_\phi) + s_\phi \tag{4.4}$$

where λ_ϕ is the diffusion coefficient and s_ϕ is the extra source/sink terms.

Using the mass conservation equation the previous generic convection-diffusion equation can also be written equivalent conv-diff equation:

$$\rho \frac{\partial \phi}{\partial t} + \rho \vec{v} \nabla \phi = \nabla \cdot (\Gamma_\phi \nabla_\phi) + s_\phi \tag{4.5}$$

Therefore, the Navier-Stokes Equations for perfect gases can be expressed in the generic convection-diffusion form:

The Navier-Stokes equations are solved integrating by the time (dt(and volume (dV) in the Control Volume (CV).

For the unsteady term:

$$\int_{t_n}^{t_{n+1}} \int_{V_p} \frac{\partial(\rho\phi)}{\partial t} dV \ dt \approx V_p \int_{t_n}^{t_{n+1}} \frac{\partial(\rho\phi)}{\partial t} dt = V_p(\rho_p\phi_p - \rho_p{}^0\phi_p{}^0)$$

For the convective term:

$$\int_{t_n}^{t_{n+1}} \int_{V_p} \nabla \cdot (\rho\vec{v}\phi)dV \ dt = \int_{t_n}^{t_{n+1}} \int_{S_f} \rho\vec{v}\phi \cdot \vec{n}dS \ dt \approx (\dot{m}_e\phi_e - \dot{m}_w\phi_w + \dot{m}_n\phi_n - \dot{m}_s\phi_s) \triangle t$$

For the diffusion term:

$$\int_{t_n}^{t_{n+1}} \int_{V_p} \nabla \cdot (\Gamma_\phi dV \ dt = \int_{t_n}^{t_{n+1}} \int_{S_f} \Gamma_\phi \nabla\phi \cdot \vec{n}dS \ dt \approx$$

$$\approx (\Gamma_e \frac{\phi_E - \phi_P}{d_{PE}} S_e - \Gamma_w \frac{\phi_P - \phi_W}{d_{PW}} S_w + \Gamma_n \frac{\phi_N - \phi_P}{d_{PN}} S_n - \Gamma_s \frac{\phi_P - \phi_S}{d_{PS}} S_s) \triangle t$$

Finally for the source term (where the source term is suposed lineal):

$$\int_{t_n}^{t_{n+1}} \int_{V_p} s_\phi dV \ dt \approx \bar{s}_{\phi p} V_p \triangle t = (S_C^\phi + S_P^\phi \phi_P) \triangle t$$

Introducing all these terms into the convection-diffusion equation:

$$\frac{\rho_p\phi_p - \rho_p{}^0\phi_p{}^0}{\triangle t} V_p + \dot{m}_e\phi_e - \dot{m}_w\phi_w + \dot{m}_n\phi_n - \dot{m}_s\phi_s =$$

$$= D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W) + D_n(\phi_N - \phi_P) - D_s(\phi_P - \phi_S) + S_C^\phi + S_P^\phi \phi_P \quad (4.6)$$

where $D_e = \Gamma_e S_e/d_{PE}$, $D_w = \Gamma_w S_w/d_{PW}$... An equivalent equation can be obtained using the discretized mass conservation equation:

$$\rho_p \frac{\phi_p - \rho_p{}^0\phi_p{}^0}{\triangle t} V_p + \dot{m}_e(\phi_e - \phi_p) - \dot{m}_w(\phi_w - \phi_p) + \dot{m}_n(\phi_n - \phi_p) - \dot{m}_s(\phi_s - \phi_p) =$$

$$= D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W) + D_n(\phi_N - \phi_P) - D_s(\phi_P - \phi_S) + S_C^\phi + S_P^\phi \phi_P \quad (4.7)$$

This equations are second-order for the diffusion and source term. However, the convective term has to be evaluated in terms of the nodal values, because it is expressed in values at the face.

4.2 Evaluations of the convective terms

There are several ways of evaluatins the convective terms:

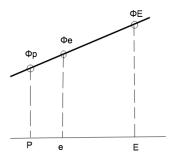### 4.2.1 Central-Difference Scheme (CDS)

Figure 4.1: Central-Difference Scheme (CDS)

It is the simplest method. It can be calculated as the average or even with the "harmonic mean" taking into account the distance from the nodes to the face.

$$\phi_e - \phi_p = f_e(\phi_E - \phi_P) \tag{4.8}$$

where the interpolation factor is:

$$f_e = d_{Pe}/d_{PE} \tag{4.9}$$

For the average method, $f_e = 1/2$. Nevertheless, CDS gives convergence problems for incompressible flows, or gases at low Mach, because the convective terms are more influenced by upstream than downstream conditions.

4.2.2 Upwind-Difference Scheme (UDS)

To solve this problem, UDS method gives more importante to the upstream condition than the downstream.

$$\phi_e - \phi_p = f_e(\phi_E - \phi_P) \tag{4.10}$$

but now:

$$f_e = 1 \quad (if \ \dot{m}_e > 0) \quad and \quad f_e = 0 \quad (if \ \dot{m}_e < 0) \tag{4.11}$$
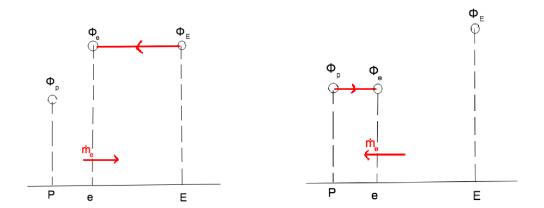
Figure 4.2: Upwind-Difference Scheme (UDS) for $\dot{m}_e > 0$

Figure 4.3: Upwind-Difference Scheme (UDS) for $\dot{m}_e < 0$

4.2.3 Exponential-Difference Scheme (EDS)

The analytical solution of the convection-diffusstion equation without the source term and for unsteady conditions can be obtained. Consideting ρ, v_x and Γ constants between nodal values and equal to the ones at the face, the equation can be integrated.

For east face:

$$\phi_e - \phi_p = f_e(\phi_E - \phi_P) \tag{4.12}$$

where:

$$f_e = \frac{e^{Pe \cdot d_{Pe}} - 1}{e^{Pe} - 1} \qquad Pe = \frac{\rho_e v_{xe} d_{PE}}{\Gamma_e} \tag{4.13}$$

Finally, the equation to solve in each node has the following structure. The same structure is found for CDS, UDS and EDS schemes.

$$a_p \cdot \phi_p = a_e \cdot \phi_e + a_w \cdot \phi_w + a_n \cdot \phi_n + a_s \cdot \phi_s + b_p$$

Where:

$$a_e = f_e \cdot \dot{m}_e - \frac{\Gamma_e}{d_{PE}} S_e \qquad a_w = -f_w \cdot \dot{m}_w - \frac{\Gamma_w}{d_{PW}} S_w$$

$$a_n = f_n \cdot \dot{m}_n - \frac{\Gamma_n}{d_{PN}} S_n \qquad a_s = -f_s \cdot \dot{m}_s - \frac{\Gamma_s}{d_{PS}} S_s$$

$$a_p = a_e + a_w + a_n + a_s - \dot{m}_e + \dot{m}_w - \dot{m}_n + \dot{m}_s \qquad b_p = 0$$

Remeber that the coefficients f_e, f_w, f_n and f_s take different values depending on the kind of scheme selected. Regularly, to simplify the nomenclature of the equations new variables are introduced (as named before):

$$F_e = \dot{m}_e \qquad D_e = \frac{\Gamma_n}{d_{PN}} S_n$$

EDS, UDS and CDS are first and second order accurate. Sometimes, it is needed more accurate schemes like a third-order or even higher. The order is related to the number of points consulted in order to establish an approximation of the value at the face.

4.2.4 Second-order Upwind Scheme (SUDS)

4.2.5 Quadratic Upwind Interpolation for convective kinematics (QUICK)

4.3 Convection-Diffussion problems

In this section, there have been developed some proposal exercises. The following exercises are steady and bidimensional, velocity field is known and density and diffussion coefficients are known constant values.

4.3.1 Parallel flow

In this problem, the velocity field is $v_x = v_0$, Inlet conditions (x=0,y): $\phi = \phi_{in}$; outlet conditions (x=L,y): $\phi = \phi_{out}$; lateral conditions (x,y = 0):$\partial \phi / \partial y = 0$.

The solution will be tested for different Peclet numbers. $Pe = \frac{\rho v_0 L}{\Gamma}$.

The analytical solutions can be obtained:

$$\frac{\phi - \phi_{in}}{\phi_{out} - \phi_{in}} = \frac{e^{xPe/L} - 1}{e^{Pe} - 1} \tag{4.14}$$

A program has been developed *CD-Lineal.cpp* (Code in *Annexes*). The following solutions have been obtained for differents Péclet numbers (-20, -10, -5, -1, 0 ,1, 5, 10, 20):
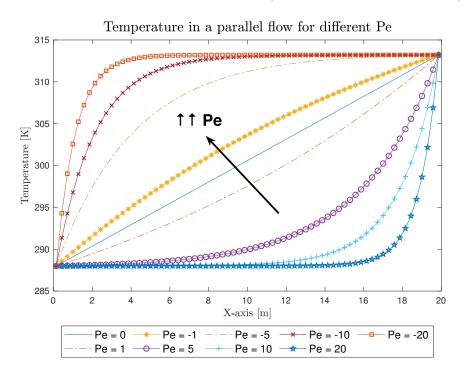

Figure 4.4: Temperature along X-axis for different Péclet Numbers

The maximum error in a point across the x-axis is approximately 0.4 %, which can be neglected. Therefore, the solution obtained and the analytical solution are consistent.

This problem has been solved as a one-dimensional (1D) problem in order to ensure that the calculations of the coefficients, parameters and the results obtained are correct. The same code has to be delevoped to bidimensional (2D) to solve the following problems.

On the other hand, in Fig. 4.5 the CDS, UDS and EDS solutions have been plotted for Pe = 1. The difference between the two of them is negligible for this Péclet number.
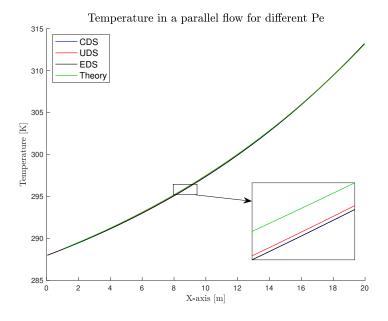

Figure 4.5: CDS , UDS & EDS solutions for Pe = 1

The Péclet number (Pe) is a dimensionless number, it is the ratio of the rate of advection of a physical quantity by the flow to the rate of diffusion of the same quantity driven by an appropriate gradient [5].

$$Pe = \frac{Advective \ \ transport \ \ rate}{Diffusive \ \ transport \ \ rate}$$

For heat transfer, the Péclet number is defined as:

$$Pe = \frac{L \cdot u}{\alpha} = Re_L \cdot Pr$$

where Pr is the Prandtl Number and Re is the Reynols Number.

4.3.2 Diagonal flow

In this case, the velocity field: $v_x = 30$; $v_y = 30$. The domain is a square region (LxL) and for number Pe = 0,6. The following solution has been obtained with UDS method Fig. 4.6. A program has been developed to obtain the solution *CD-Diagonal.cpp* (Code in *Annexes*).
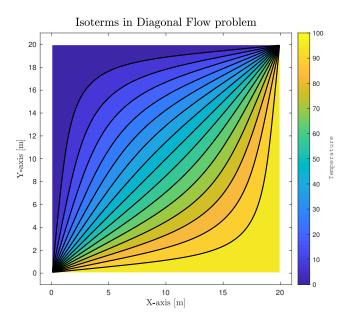

Figure 4.6: Isotherms in a Diagonal Flow

Furthermore, for Pe $= \infty$ using UDS method Fig. 4.7.As observed, the solution can be divided into two regions. The upper diagonal part in which the temperature (ϕ) achieves the value of ϕ_{LOW} and the lower diagonal part, the temperature corresponds to ϕ_{HIGH}. The increase the width of the diagonal is due to the fact that UDS has been used, and it doesn't take into account the previous terms if the mass flow is pointing towards the positive direction of axis x and y.
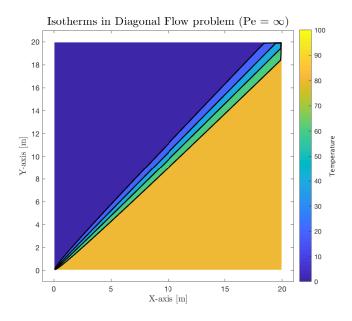
Figure 4.7: Isotherms in a Diagonal Flow ($Pe = \infty$)

4.3.3 Smith-Hutton problem

This problem was proposed by R.M. Smith and A.G. Hutton in 1982. Smith-Hutton problem is a test problem which permits the evaluation of different numerical schemes (first order, second order, third or higher orders).

The problems consists in a rectangular region (2LxL), with one inlet and one outlet [7]. The stream function Ψ is known, therefore the velocity field of the fluid is also known.

$$\Psi = (1 - x^2) \cdot (1 - y^2)$$

$$u(x,y) = \frac{\partial \Psi}{\partial y} = 2y(1 - x^2) \qquad v(x,y) = -\frac{\partial \Psi}{\partial x} = -2x(1 - y^2)$$

All boundary conditions are Dirichlet, except for the boundary at the outlet wall that is Neummann boundary condition.

$$\phi = 1 + tanh(\alpha(2x + 1)) \qquad (for\ y = 0;\ -1 < x < 0) \quad (Inlet flow)$$

$$\frac{\partial \phi}{\partial y} = 0 \qquad (for\ y = 0;\ 0 < x < 1) \quad (Outlet\ flow)$$

$$\phi = 1 + tanh(\alpha) \qquad (for\ the\ rest\ of\ walls)$$

In this case, $\alpha = 10$. The solution has been done for different ratios of ρ/Γ, that indicates a ratio between the diffusive and convective term. A program has been developed to obtain the solution *CD-SmithHutton.cpp* (Code in *Annexes*).
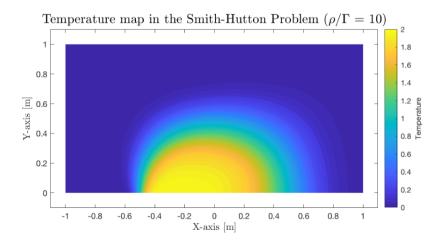

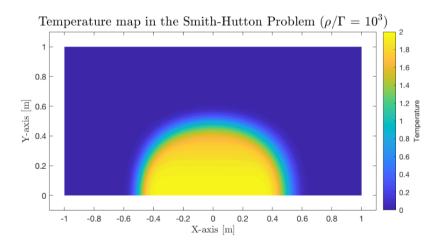Figure 4.8: Solution of Smith-Hutton problem for Pe $= 10$

Figure 4.9: Solution of Smith-Hutton problem for Pe $= 10^3$

In order to solve Convection-Diffusion incompressible and steady problems the sequence of actions and calculations are resumed in Fig. 4.11.
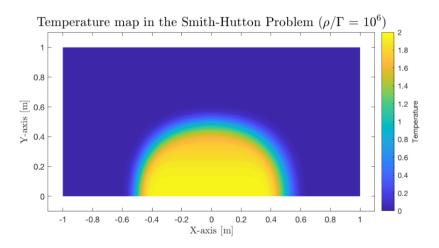
4.4   Summary

Figure 4.10: Solution of Smith-Hutton problem for Pe $= 10^6$

	$\frac{\rho}{\Gamma} = 10$		$\frac{\rho}{\Gamma} = 10^3$		$\frac{\rho}{\Gamma} = 10^6$	
x-position	ϕ_{theo}	ϕ_{exp}	ϕ_{theo}	ϕ_{exp}	ϕ_{theo}	ϕ_{exp}
0.0	1.989	1.9880	2.0000	2.0000	2.000	2.000
0.1	1.402		1.9990	1.9992	2.000	2.000
0.2	1.146		1.9997	1.9983	2.000	2.000
0.3	0.946		1.9850	1.9955	1.999	2.000
0.4	0.775		1.8410	0.9737	1.964	1.983
0.5	0.621		0.9510	0.9737	1.000	0.959
0.6	0.480		0.1540	0.0950	0.036	0.089
0.7	0.349		0.0010	0.0024	0.001	0.002
0.8	0.227		0.0000		0.000	0.000
0.9	0.111		0.0000	0.0000	0.000	0.000
1.0	0.000		0.0000	0.0000	0.000	0.000

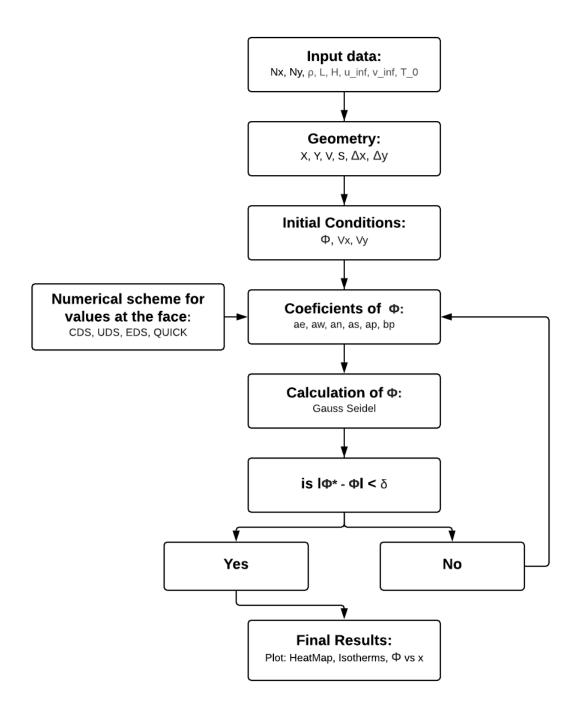Table 4.2: Comparison between obtained results for different $\frac{\rho}{\Gamma}$ ratios

Figure 4.11: Diagram solution of steady Convection-Diffusion problems

5 Navier-Stokes

On this chapter there will be developed a solution of Navier-Stokes for the Driven Cavity case.

5.1 Fractional Step Method (FSM)

The Fractional Step Method is common technique for solving NS equations. The Navier-Stokes equations for incompressible and constant viscosity flows are:

$$\nabla \cdot (\rho \vec{v} = 0$$

$$\rho \frac{\vec{v}}{\partial t} + (\rho \vec{v} \cdot \nabla)\vec{v} = -\nabla p + \mu \nabla \vec{v}$$

Introducing the new term R, the momentum equation can be written as:

$$\rho \frac{\vec{v}}{\partial t} = \mathbf{R}(\vec{v}) - \nabla p \tag{5.1}$$

where, $\mathbf{R}(\vec{v}) = -(\rho \vec{v} \cdot \nabla)\vec{v} + \mu \nabla \vec{v}$.

Time intregration of NS equations are:

$$\nabla \cdot (\rho \vec{v}^{n+1} = 0 \tag{5.2}$$

For time integration of the convective-diffusive term Adams-Bashforth scheme is used:

$$\rho \frac{\vec{v}^{n+1} - \vec{v}^n}{\delta t} = \frac{3}{2}\mathbf{R}(\vec{v}^n) - \frac{1}{2}\mathbf{R}(\vec{v}^{n+1}) - \nabla p^{n+1} \tag{5.3}$$

Momentum equations are integrated at time instant (n+1/2) while continuity equations is implicitly integrated.

Now, it will be introduced a unique decomposition (thanks to the Helmholtz-Hodge theorem). The theorem establishes that a given A and given vector field ω, defined in a bounded domain Ω with smooth boundary $\Delta\Omega$, is uniquely decomposed in a pure gradient field and a divergence-free vector parallel to $\Delta\Omega$.

$$\vec{\omega} = \vec{a} + \nabla\phi$$

where, $\nabla\vec{a} = 0$ for a Ω. The theorem also applies for periodic inflow/outflow conditions.

Introducing the HH theorem into Eq.5.1, an equation for pressure can be derived from the velocity decomposition equations if the divergence operator is applied:

$$\nabla \vec{v}^{n+1} = \nabla \vec{v}^p - \nabla \cdot (\frac{t}{\rho} \nabla p^{n+1})$$

Since $\nabla \vec{v}^{n+1} = 0$, finally a Poisson equation for the pressure is found:

$$\nabla p^{n+1} = \frac{\rho}{t} \nabla \cdot \vec{v}^p$$

Finally, v^{n+1} results from the original decomposition:

$$\vec{v}^{n+1} = \vec{v}^p - \frac{t}{\rho} \nabla p^{n+1}$$

Therefore, at each time step the following equations give a unique $\vec{v}^{n+1}$ and ∇p^{n+1}. The FSM can be resumed in these steps:

1. Evaluation of $\mathbf{R}(\vec{v})^n)$

2. Evaluate the predictor velocity $(\vec{v})^p)$, using the convective-diffusive temrs of the previous step: $(\vec{v})^p) = (\vec{v})^n) + \frac{t}{\rho}[3/2\mathbf{R}(\vec{v})^n) - 1/2\mathbf{R}(\vec{v})^{n+1})]$

3. Solve Poisson equation to obtain the pressure: $\nabla p^{n+1} = \frac{\rho}{t} \nabla \vec{v}^p$

4. Obtain the velocity field: $\vec{v}^{n+1} = \vec{v}^p - \frac{t}{\rho} \nabla p^{n+1}$

5. Choose the new $t = \min (t_c, t_d)$

5.1.1 Checkerboard problem

A checker board problem arises due to the nature of the central difference scheme when applied to the divergence operator and the pressure gradient operator.

The calculation of the pressure gradient only depends on the pressure surrounding nodes, but not the node it self. This could give unrealistic pressure fields, eventhough a realistic and stable velocity field is obtained.

There are two possibilities to solve this problem:

- Collocated mesh

  In the collocated mesh in Cartesian coordinates velocity components (u, v, w) are stored with the pressure p at the cell center [8].

  An interpolation of the velocity value at the wall has to be interpolated through interpolation of the cell-centered values plus a projection operation that guarantees exact conservation of mass [9].

- Staggered mesh

  In a staggered mesh, one mesh is created for the pressure field and another for the velocity field [8, 10].

In this case, for velocity field $\vec{v} = (u, v)$ it will be used a staggered mesh in order to avoid the checkerboard problem.

On a staggered grid the scalar variables (pressure, density, total enthalpy etc.) are stored in the cell centers of the control volumes, whereas the velocity or momentum variables are located at the cell faces. A staggered storage is mainly used on structured grids for compressible or incompressible flow simulations.

Figure 5.1: Collocated and Staggered Meshes

Using a staggered grid (Fig.**??**) is a simple way to avoid odd-even decoupling [**OddsEvens**] between the pressure and velocity. Odd-even decoupling is a discretization error that can occur on collocated grids and which leads to checkerboard patterns in the solutions.

The disadvantage of using staggered grids is that different variable are stored at different places and this makes it more difficult to handle different control volumes for different varibales and to keep track of the metrics. Most modern codes instead use a collocated storage. [**Stagg**]

The FSM is achieved at each time step and finishes when the steady state is reached.

5.2   Time step determination

According to CFL (Courant-Friedrich-Levy) condition, the mininum time for convective and for diffussive term are:

$$t_c = min(0.35 \, \frac{x}{\vec{v}}) \tag{5.4}$$

$$t_d = min(0.20 \, \frac{\rho x^2}{\mu}) \tag{5.5}$$

$$t = min(t_c, t_d)$$

The predictor velocity provides an approximate solution of the momentum equations, but it cannot satisfy the incompressibility constraint. The Poisson equation for pressure [11] determines the minimum perturbation that will make the predictor velocity incompressible.
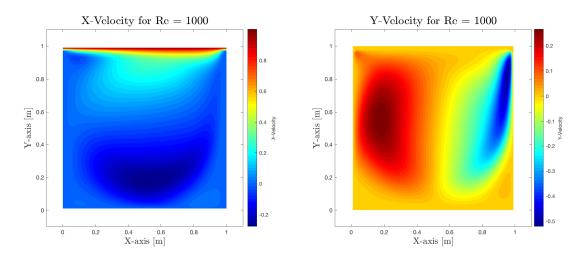
5.3   Driven Cavity

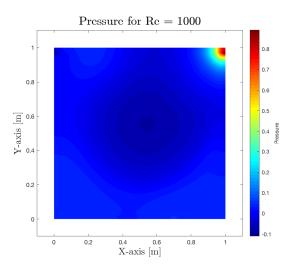Figure 5.2: X-velocity for Re = 1000

Figure 5.3: Y-velocity for Re=1000

Figure 5.4: Pressure for Re = 1000

5.4   Summary

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