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Study for the computational resolution of conservation equations of mass, momentum and energy. Possible application to different aeronautical and industrial engineering problems: Case 1B

Report

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Part I

Introduction

1 | Introduction

1.1 Aim

The main objective of this paper is to provide knowledge in the computational resolution of the fundamental equations of fluid dynamics and mass and heat transfer by developing simulation codes. A second objective would be to apply the developed and verified codes in a specific case.

1.2 Scope

First, some basic cases concerning the equations of mass, momentum and energy are going to be solved in order to learn the fundamentals of the mathematical formulation and the computational and programming techniques that are going to be needed to develop the whole study. With the help of these cases, some simulation codes are going to be developed.

A second part of this paper is going to be the application of the knowledge acquired to a practical case, that may be an engineering system or any other physical system.

In order to accomplish the objectives mentioned above, these are the following tasks to be developed:

- Previous research of the state of the art.
- Theoretical approach of the fluid dynamics behind all the cases and study of the mathematical formulation that should be applied.
- Development of the necessary numerical simulation tools. All the codes will need to be validated to ensure they are correct.
- Application of the acquired knowledge in simulation codes to an specific system.

- Analysis of the results.
- Conclusions.

1.3 Requirements

- Codes must be developed in C or C++.
- No external libraries or solvers can be used.
- Codes must be in a single file and compile with no errors.
- Codes must run without any input.
- Codes should be able to be executed in a normal computer.
- Simulations should provide realistic results.

Finally, there are no economical or legal requirements because the software used for this study is completely open source.

1.4 Justification

1.4.1 Identification of the need

Conservation equations of mass, momentum and energy define the motion of fluids. Most thermal and engineering problems require to solve these equations to achieve the desired result. However, they are coupled differential equations, which means they are difficult to solve. Except for a few simplified cases, they usually do not have an analytical solution, so a numerical approach is often necessary. A huge amount of cases have been solved in the recent years, but there are still other problems that need to be studied and developed.

Since these equations need for a numerical resolution in the majority of cases, the knowledge of computational techniques is essential to improve the simulations in accuracy and efficiency. A better understanding on the computational resolution of the conservation equations can lead to better results in the numerical simulations and with less computational cost. As a consequence, the actual knowledge in a variety of subjects could be improved, such as the temperature variation inside an engine or the way the air moves in the respiratory system. Furthermore, it could also lead to an optimization of different engineering systems; for example, more efficient wings for future airplanes.

1.4.2 Advantages and drawbacks

The main advantage of the approach explained in the scope is that the study of the computational resolution is started from basic cases and its difficulty is upgraded with every case of fluid dynamics that is proposed. That way, the comprehension on the developed simulations is higher, which makes the codes more reliable. However, the simulation codes are being developed from zero. This is an advantage because no previous errors are going to be introduced on the program, but it is also a drawback because its development could take some time.

Anyhow, this project can be useful in the study of new engineering and thermal problems that need to be solved using the conservation equations of mass, momentum and energy; and can lead to other new studies of computational resolution of these equations.

Part II

Numerical analysis

2 | Numerical methods

The laws governing the processes of heat transfer and fluid flow are usually expressed in terms of differential equations. Some of these equations are the momentum equation, the energy equation and the mass conservation equation, among others. However, these expressions usually don't have an analytical solution except for some simple cases. To solve complex problems it is necessary to use numerical methods.

2.1 Conservation equations

The three most important conservation equations are the mass conservation equation, the momentum conservation equation and the energy conservation equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (2.1)$$

$$\frac{\partial}{\partial t} (\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot \vec{r} + \rho \vec{g} + \vec{f}^e \quad (2.2)$$

$$\frac{\partial}{\partial t} (\rho u) + \nabla \cdot (\rho \vec{v} u) = -\nabla \cdot \vec{q} - p \nabla \cdot \vec{v} + \vec{r} : \nabla \vec{v} + \Phi^e \quad (2.3)$$

For incompressible flows with no viscous dissipation, the energy conservation equation can be written as:

$$\rho c_p \left(\frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T \right) = \nabla \cdot (\lambda \nabla T) \quad (2.4)$$

All these equations can be seen as a particular case of the generic convection-diffusion equation:

$$\frac{\partial}{\partial t} (\rho \phi) + \nabla \cdot (\rho \vec{v} \phi) = \nabla \cdot (\Gamma \nabla \phi) + S_{phi} \quad (2.5)$$

where ρ is the density, \vec{v} the velocity, Γ the diffusion coefficient, S_ϕ the source term, and ϕ the general variable that is going to be studied. Some examples can be found in table 2.1.

Equation	ϕ	Γ	S_ϕ
Mass conservation	1	0	0
Momentum	\vec{v}	μ	$-\nabla p + \nabla \cdot \vec{r} + \rho \vec{g} + \vec{f}^e$
Energy (for a semiperfect gas)	u	λ/c_v	$-\nabla \cdot \vec{q} - p \nabla \cdot \vec{v} + \vec{r} : \nabla \vec{v} + \Phi^e$

Table 2.1: Particular cases of the convection-diffusion equation

2.2 Numerical methods

Numerical methods are based in dividing the domain that is going to be studied in different pieces. Instead of calculating the unknowns in the whole domain, they are studied in the finite number of points defined by these pieces, the grid points. This process is called discretization. Once the domain is discretized, it is also necessary to discretize the equations. The relations between the grid points have to be established. It is assumed that the value ϕ of a grid point only influences the distribution of ϕ in its immediate neighbours. For this reason, as the number of grid points becomes larger, the numerical solution approaches the real solution of the problem. There are different methods of discretizing the equations, but the most common ones are exposed in the following lines.

2.3 Finite difference method

The finite difference method (FDM) is based in the Taylor-series expansion. It is used to approximate the derivatives in the differential equation. Taking the three successive points represented in figure 2.1, the approximation of the values in the left point (west) and in the right point (east) is easily calculated with Taylor series:

$$\phi_W = \phi_P - \Delta x \left(\frac{d\phi}{dx} \right)_P + \frac{1}{2} (\Delta x)^2 \left(\frac{d^2\phi}{dx^2} \right) - \dots \quad (2.6)$$

$$\phi_E = \phi_P + \Delta x \left(\frac{d\phi}{dx} \right)_P + \frac{1}{2} (\Delta x)^2 \left(\frac{d^2\phi}{dx^2} \right) + \dots \quad (2.7)$$

Using a second order approximation and combining both expressions, it can be easily obtained:

$$\left(\frac{d\phi}{dx} \right)_P \approx \frac{\phi_E - \phi_W}{2\Delta x} \quad (2.8)$$

$$\left(\frac{d^2\phi}{dx^2} \right)_P \approx \frac{\phi_W + \phi_E - 2\phi_P}{(\Delta x)^2} \quad (2.9)$$

These expressions are substituted in the differential equation to obtain the finite-differential equation. This approach is very simple, but it is not used in complex geometries. It also does not enforce the conservation, as it is simply a mathematical approach, which may lead to some problems.

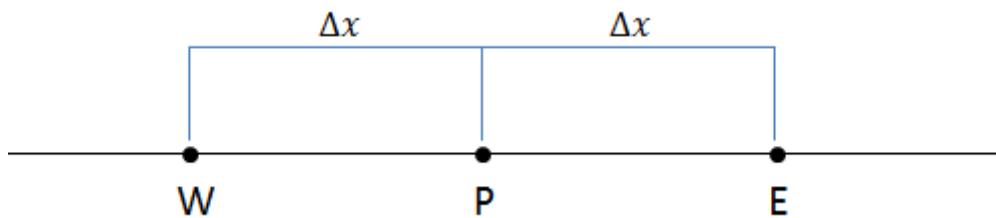


Figure 2.1: Three successive grid points

2.4 Finite volume method

The finite-volume method (FVM) is more used than the FDM. It consists in dividing the domain in different control volumes as the ones in figure 2.2, so that each control volume surrounds one grid point. Then, the differential equation is integrated over each control volume, ensuring that each of them satisfy the conservation.

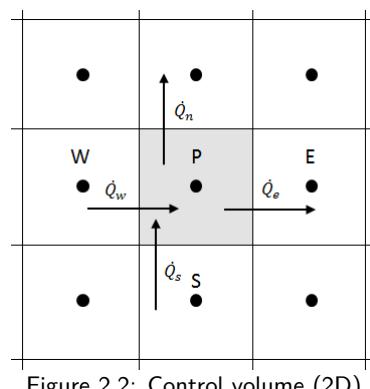


Figure 2.2: Control volume (2D)

2.4.1 Mesh

There are different methods to divide discretize the domain for the FVM. These methods are listed below [1]:

- Structured (regular) mesh: The grid lines do not cross each other. The lines can be numbered consecutively, so as the position of any grid point can be easily identified by two (2D) or three (3D) indices. This is the simplest structure and easiest to work with, but it can only be used for geometrically simple domains.
- Unstructured mesh: The control volumes may have any shape, and there is not a restriction on the number of neighbour nodes. It is the method used for very complex geometries, but the grid generation and the pre-processing are much difficult than on structured meshes.

2.5 Time integration

Time is a one-way variable, which means that the unknowns only depend on the values in the previous instant of time, and do not depend on the values in the next instant of time. Taking this property into account, to obtain the results of an unsteady problem, the method is to discretize the time and calculate the values for each time step. When the unknowns of one time step are obtained, the calculation moves on to the next time step.

Time integration can be done using different methods. The ones that are widely used are:

- Explicit method: The simplest method. All the terms are evaluated using the known values of the previous time step t^n . It is a first order approximation and easy to compute, but it requires very small time steps in order to achieve convergence.
- Implicit method: It is a very stable first order approximation, useful in problems with large time steps. The terms are evaluated with the values in the next instant of time t^{n+1} .
- Crank-Nicholson: It is a second order approximation. The terms are evaluated using the values of the previous and the next time step.

2.6 Interpolation schemes

In some cases, it is necessary to obtain the properties of the points that are not nodes. Usually, a term is evaluated in the faces, not in the nodes, so it is necessary to know the values in the faces of the control volume. There are different schemes to do so. Some of the most common ones are listed below [1, 2].

2.6.1 The central differencing scheme (CDS)

It is the most natural scheme. It is a linear interpolation between the two nearest nodes:

$$\phi_e - \phi_P = \frac{d_{Pe}}{d_{PE}} (\phi_E - \phi_P) \quad (2.10)$$

However, CDS is only valid in cases with low Reynolds number. It is a second order approximation, but may produce oscillatory solutions.

2.6.2 The upwind scheme (UDS)

It assumes that the value of ϕ in the interface is equal to the value of ϕ at the node on the upwind side of the face.

$$\begin{aligned}\phi_e &= \phi_P, & \text{if } \dot{m}_e > 0 \\ \phi_e &= \phi_E, & \text{if } \dot{m}_e < 0\end{aligned}\tag{2.11}$$

The solutions of the UDS will always be physically realistic, but they may not be completely accurate because it is a first order approximation. However, this method is widely used because of its stability.

2.6.3 The exponential scheme (EDS)

Taking the generic convection-diffusion equation and assuming a steady one-dimensional problem with a constant Γ and no source term, the analytic solution of the equation is an exponential function:

$$\frac{\phi - \phi_0}{\phi_L - \phi_0} = \frac{\exp(Px/L) - 1}{\exp(P) - 1}\tag{2.12}$$

Where ϕ_0 and ϕ_L are the values of the function at $x = 0$ and $x = L$ respectively and P is the Péclet number, a non-dimensional number:

$$P \equiv \frac{\rho u L}{\Gamma}\tag{2.13}$$

In the EDS, this analytic solution is used to determine the value on the faces, using the following expression:

$$\phi_e - \phi_P = \frac{\exp(P_e d_{Pe}/d_{PE}) - 1}{\exp(P_e) - 1} (\phi_E - \phi_P)\tag{2.14}$$

Though this solution is exact for the steady one-dimensional problem it is not for two or three-dimensional cases, unsteady problems... so it is not widely used.

2.6.4 The hybrid scheme (HDS) and the power-law scheme (PLDS)

Both methods are an approximation of the exponential function used in the EDS. Since exponentials are expensive to compute, the HDS and the PLDS are meant to provide a good result but with simpler functions. They divide the function given by the EDS in different parts and approximate the solution with simpler functions.

Part III

Conduction

3 | Conduction

Conduction refers to the heat transfer through a solid or a stationary fluid [3]. It occurs due to the difference of temperatures between the different parts of the solid, that generates a heat flux from the area with higher temperature to the one with lower temperature. It depends on the temperature gradient and the physical properties of the material.

3.1 Governing equations

The conduction heat transfer in a solid is described by equation 3.1:

$$\rho c_P \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + \dot{q}_v \quad (3.1)$$

Where ρ is the density of the material, T the temperature, λ its conductivity, c_P its specific heat and \dot{q}_v its inner heat (source term).

The heat transfer \vec{q} between two points in the direction \vec{n} is described with the Fourier law 3.2:

$$\vec{q} = -\lambda \frac{\partial T}{\partial n} \vec{n} \quad (3.2)$$

3.2 Discretization

To discretize the equation, the finite volume method is used, dividing the domain with a Cartesian grid. The domain is discretized using the node centred distribution, to avoid having conflictive control volumes between the different materials.

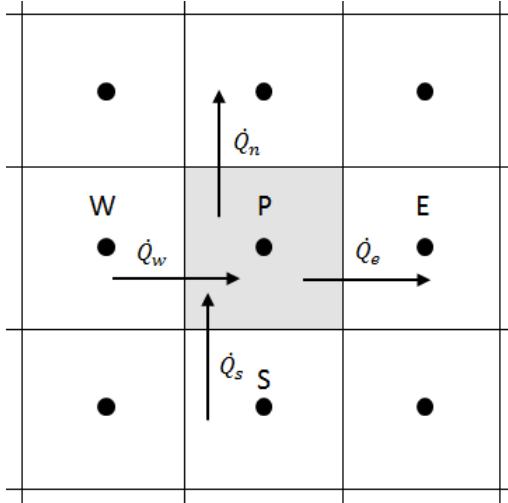


Figure 3.1: Heat fluxes through the faces of a control volume

3.2.1 Spatial discretization

The heat fluxes through the walls represented in figure 3.1 are defined by equation 3.2. They are obtained integrating the expression in the vertical and horizontal directions.

$$\dot{Q}_e = - \int^{S_e} \lambda \frac{\partial T}{\partial x} dS \approx - \left(\lambda \frac{\partial T}{\partial x} \right)_e S_e \approx -\lambda_e \frac{T_E - T_P}{d_{PE}} S_e \quad (3.3)$$

$$\dot{Q}_w = - \int^{S_w} \lambda \frac{\partial T}{\partial x} dS \approx - \left(\lambda \frac{\partial T}{\partial x} \right)_w S_w \approx -\lambda_w \frac{T_P - T_W}{d_{PW}} S_w \quad (3.4)$$

$$\dot{Q}_n = - \int^{S_n} \lambda \frac{\partial T}{\partial x} dS \approx - \left(\lambda \frac{\partial T}{\partial x} \right)_n S_n \approx -\lambda_n \frac{T_N - T_P}{d_{PN}} S_n \quad (3.5)$$

$$\dot{Q}_s = - \int^{S_s} \lambda \frac{\partial T}{\partial x} dS \approx - \left(\lambda \frac{\partial T}{\partial x} \right)_s S_s \approx -\lambda_s \frac{T_P - T_S}{d_{PS}} S_s \quad (3.6)$$

where T is the temperature at the given node, d the distance between two nodes, and λ the conductivity at the given face.

The inner heat of the material can be discretized as:

$$Q_{VP} = \int_{V_P} \dot{q}_v dV \approx \dot{q}_{VP} V_P \quad (3.7)$$

In the heat fluxes, though, the conductivity can have two different values: one on the left node and another one on the right node. Taking the value of the conductivity of just one node could lead to non-realistic results, because the heat fluxes evaluate the gradient of temperatures from one node to the other. To avoid this problem, the conductivity is determined using the harmonic mean 3.11. This solution is justified operating the heat fluxes through the wall:

$$\dot{q}_e^- = \dot{q}_e^+ \quad (3.8)$$

$$-\lambda_P \frac{T_e - T_P}{d_{Pe}} = -\lambda_E \frac{T_E - T_e}{d_{Ee}} \quad (3.9)$$

$$\dot{q}_e = -\lambda_e \frac{T_E - T_P}{d_{PE}} \quad (3.10)$$

$$\lambda_e = \frac{d_{PE}}{\frac{d_{Pe}}{\lambda_P} + \frac{d_{Ee}}{\lambda_E}} \quad (3.11)$$

3.2.2 Temporal discretization

The time discretization is done using the First law of thermodynamics:

$$\int_{V_P} \rho \frac{\partial u}{\partial t} dV = \sum \dot{Q}_P \quad (3.12)$$

where u is the internal energy of the control volume. Assuming an incompressible material, the First law of thermodynamics is integrated over time. Taking n as the previous instant of time and $n + 1$ the instant of time that is going to be calculated:

$$\int_{t^n}^{t^{n+1}} \rho_P \frac{\partial \bar{u}_P}{\partial t} V_P dt = \int_{t^n}^{t^{n+1}} \sum \dot{Q}_P dt \quad (3.13)$$

Rearranging the first term of the equation:

$$\begin{aligned} \int_{t^n}^{t^{n+1}} \rho_P \frac{\partial \bar{u}_P}{\partial t} V_P dt &= \rho_P V_P (\bar{u}_P^{n+1} - \bar{u}_P^n) \approx \\ &\rho_P V_P (u_P^{n+1} - u_P^n) = \rho_P V_P \bar{c}_P (T_P^{n+1} - T_P^n) \end{aligned} \quad (3.14)$$

To integrate the second term of the equation over time, a new variable β is introduced, so as to be able to use an implicit, explicit or Crank-Nicholson scheme as explained in section 2.5.

$$\int_{t^n}^{t^{n+1}} \sum \dot{Q}_P dt = [\beta \sum \dot{Q}_P^{n+1} + (1 - \beta) \sum \dot{Q}_P^n] \Delta t \quad (3.15)$$

The discretized equation is finally obtained as the sum of both terms:

$$\rho_P V_P \bar{c}_P \frac{T_P^{n+1} - T_P^n}{\Delta t} = \beta \sum \dot{Q}_P^{n+1} + (1 - \beta) \sum \dot{Q}_P^n \quad (3.16)$$

where

$$\begin{aligned} \dot{Q}_P &= -\dot{Q}_w + \dot{Q}_e - \dot{Q}_s + \dot{Q}_n + \dot{q}_{vP} V_P = \\ &- \lambda_w \frac{T_P - T_W}{d_{PW}} S_w + \lambda_e \frac{T_E - T_P}{d_{PE}} S_e - \lambda_s \frac{T_P - T_S}{d_{PS}} S_s + \lambda_n \frac{T_N - T_P}{d_{PN}} S_n + \dot{q}_{vP} V_P \end{aligned} \quad (3.17)$$

To simplify the equation, it can be rewritten with coefficients, dependant on the properties of the nearest nodes in the following form:

$$a_P T_P = a_E T_E + a_W T_W + a_N T_N + a_S T_S + b_P \quad (3.18)$$

The coefficients are called discretization coefficients, and they are different for each node. The discretization coefficients are:

$$a_E = \beta \frac{\lambda_e S_e}{d_{PE}} \quad (3.19)$$

$$a_W = \beta \frac{\lambda_w S_w}{d_{PW}} \quad (3.20)$$

$$a_N = \beta \frac{\lambda_n S_n}{d_{PN}} \quad (3.21)$$

$$a_S = \beta \frac{\lambda_s S_s}{d_{PS}} \quad (3.22)$$

$$a_P = a_E + a_W + a_N + a_S + \rho_P V_P \bar{c}_P / \Delta t \quad (3.23)$$

$$\begin{aligned} b_P = & \frac{\rho_P V_P \bar{c}_P T_P^n}{\Delta t} + \beta \dot{q}_{vP}^{n+1} V_P + \\ & (1 - \beta) \left[-\lambda_w \frac{T_P - T_W}{d_{PW}} S_w + \lambda_e \frac{T_E - T_P}{d_{PE}} S_e - \lambda_s \frac{T_P - T_S}{d_{PS}} S_s + \lambda_n \frac{T_N - T_P}{d_{PN}} S_n + \dot{q}_{vP} V_P \right]^n \end{aligned} \quad (3.24)$$

3.3 Boundary conditions

There are three kinds of boundary conditions that are common in conduction problems [3]:

- Constant surface temperature: The temperature of a surface is prescribed. The condition is fulfilled just by substituting the value of the prescribed temperature in the conduction equation.

$$T_{wall} = T_{prescribed} \quad (3.25)$$

- Constant surface heat flux: The heat flux in a surface is prescribed. In some cases the surface is adiabatic, which means $\dot{q} = 0$. In this case, the condition is imposed just by adding the heat flux to the conduction equation.

$$\dot{q}_{wall} = \dot{q}_{prescribed} \quad (3.26)$$

- Convection surface condition: This boundary condition refers to the existence of convection heat transfer at the surface. To fulfil this condition, it is necessary to calculate the heat transfer due to the convection:

$$\dot{q}_{conduction} = -\lambda \frac{T_{node} - T_{wall}}{d_{nw}} \quad (3.27)$$

$$\dot{q}_{convection} = \alpha (T_g - T_{wall}) \quad (3.28)$$

$$\dot{q}_{conduction} = \dot{q}_{convection} \quad (3.29)$$

$$\dot{q} = \frac{T_g - T_{node}}{\frac{1}{\alpha} + \frac{d_{nw}}{\lambda}} \quad (3.30)$$

where T_g is the temperature of the fluid next to the wall, α the convection heat transfer coefficient, T_{node} the temperature of the node next to the wall, and d_{nw} the distance from the node to the wall.

4 | A Two-dimensional Transient Conduction Problem

The four materials problem is a two-dimensional transient conduction problem. It consists in a long rod composed of four different materials with different properties. The general scheme of the problem is represented in figure 4.1, and the dimensions of the materials, their properties, and the boundary conditions are in the tables below.

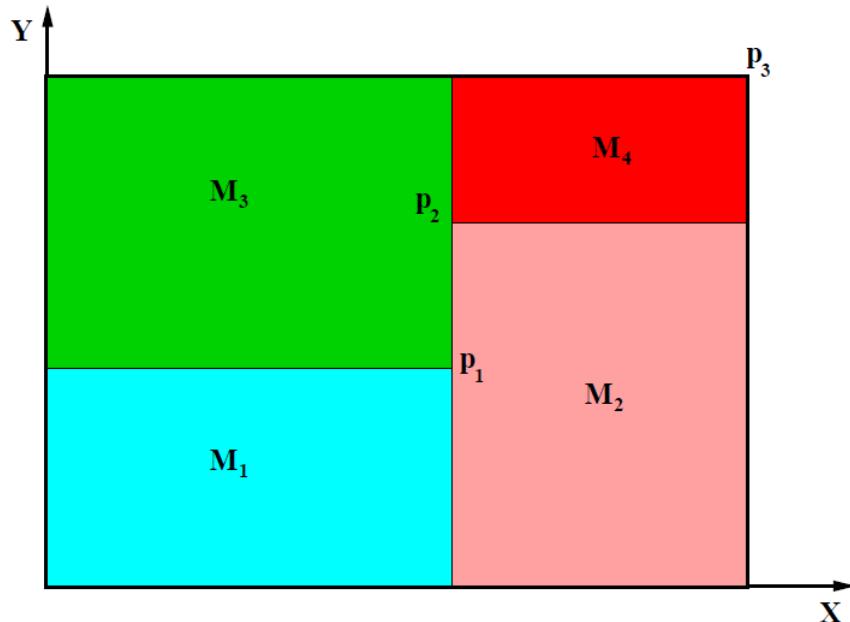


Figure 4.1: General scheme of the four materials problem

	x [m]	y [m]
p ₁	0.50	0.40
p ₂	0.50	0.70
p ₃	1.10	0.80

Table 4.1: Problem coordinates

	$\rho [kg/m^3]$	$c_P [J/kgK]$	$\lambda [W/mK]$
M_1	1500.00	750.00	170.00
M_2	1600.00	770.00	140.00
M_3	1900.00	810.00	200.00
M_4	2500.00	930.00	140.00

Table 4.2: Physical properties of the materials

Cavity wall	Boundary condition
Bottom	Isotherm at $T = 23.00^\circ C$
Top	Uniform $Q_{flow} = 60.00 W/m$ length
Left	In contact with a fluid at $T_g = 33.00^\circ C$ and heat transfer coefficient $9.00 W/m^2 K$
Right	Uniform temperature $T = 8.00 + 0.005t^\circ C$ (where t is the time in seconds)

Table 4.3: Boundary conditions

The initial temperature field is $T = 8.00^\circ C$.

4.1 Discretization

The spatial discretization of the problem is that described in section 3.2.1. However, since there are different materials, each of them is discretized separately. The variable M_1 is the number of control volumes in the vertical direction from $Y = 0$ to the point p_1 , M_2 from p_1 to p_2 and M_3 from p_2 to p_3 . In the horizontal direction, the variable N_1 is the number of control volumes from $X = 0$ to the point p_1 and N_2 from p_1 to p_3 .

M_1	M_2	M_3	N_1	N_2	δ
40	30	10	50	60	10^{-3}

Table 4.4: Numerical parameters of the four materials problem

4.2 Boundary conditions

The coefficients of the discretized equation in the inner nodes are the ones of the section 3.2.2. The outer walls of the rod have special conditions, so each of them has to be studied in order to determine which coefficients of their boundary nodes are different.

In the left wall, there is convection with the fluid outside of the road. In order to fulfil this condition, some coefficients have to be recalculated:

$$a_W = 0 \quad (4.1)$$

Boundary conditions

$$a_P = a_E + a_W + a_N + a_S + \frac{\rho_P V_P \bar{c}_P}{\Delta t} + \beta \frac{\frac{1}{\alpha} + \frac{d_{Pw}}{\lambda_P}}{1 + \frac{d_{Pw}}{\lambda_P}} \quad (4.2)$$

$$\begin{aligned} b_P &= \frac{\rho_P V_P \bar{c}_P T_P^n}{\Delta t} + \beta \left(\dot{q}_{vP}^{n+1} V_P + \frac{T_g}{\frac{1}{\alpha} + \frac{d_{Pw}}{\lambda_P}} \right) \\ &+ (1 - \beta) \left[\frac{T_g - T_P}{\frac{1}{\alpha} + \frac{d_{Pw}}{\lambda_P}} + \lambda_e \frac{T_E - T_P}{d_{PE}} S_e - \lambda_s \frac{T_P - T_S}{d_{PS}} S_s + \lambda_n \frac{T_N - T_P}{d_{PN}} S_n + \dot{q}_{vP} V_P \right]^n \end{aligned} \quad (4.3)$$

There is a constant heat flux in the top wall. The value of this flux is given for the total wall, so it is assumed that it is uniformly distributed over the top wall. In this case, the coefficients that change their value are:

$$a_N = 0 \quad (4.4)$$

$$\begin{aligned} b_P &= \frac{\rho_P V_P \bar{c}_P T_P^n}{\Delta t} + \beta \dot{q}_{vP}^{n+1} V_P + Q_{flow} \frac{S_n}{S_{top}} \\ &+ (1 - \beta) \left[-\lambda_w \frac{T_P - T_W}{d_{PW}} S_w + \lambda_e \frac{T_E - T_P}{d_{PE}} S_e - \lambda_s \frac{T_P - T_S}{d_{PS}} S_s + \dot{q}_{vP} V_P \right]^n \end{aligned} \quad (4.5)$$

In the right wall, the temperature T_r is given, and it changes over time. The coefficients are very similar to those of the general case. The only differences are:

$$a_E = 0 \quad (4.6)$$

$$a_P = a_E + a_W + a_N + a_S + \frac{\rho_P V_P \bar{c}_P}{\Delta t} + \beta \frac{\lambda_P S_e}{d_{Pe}} \quad (4.7)$$

$$\begin{aligned} b_P &= \frac{\rho_P V_P \bar{c}_P T_P^n}{\Delta t} + \beta \left(\dot{q}_{vP}^{n+1} V_P + \frac{\lambda_P S_e}{d_{Pe}} T_r^{n+1} \right) \\ &+ (1 - \beta) \left[-\lambda_w \frac{T_P - T_W}{d_{PW}} S_w + \lambda_P \frac{T_r - T_P}{d_{Pe}} S_e - \lambda_s \frac{T_P - T_S}{d_{PS}} S_s + \lambda_n \frac{T_N - T_P}{d_{PN}} S_n + \dot{q}_{vP} V_P \right]^n \end{aligned} \quad (4.8)$$

Finally, in the bottom wall, the temperature T_b is also given, but it is constant over time. The approach is very similar to that of the right wall, so that the different coefficients are:

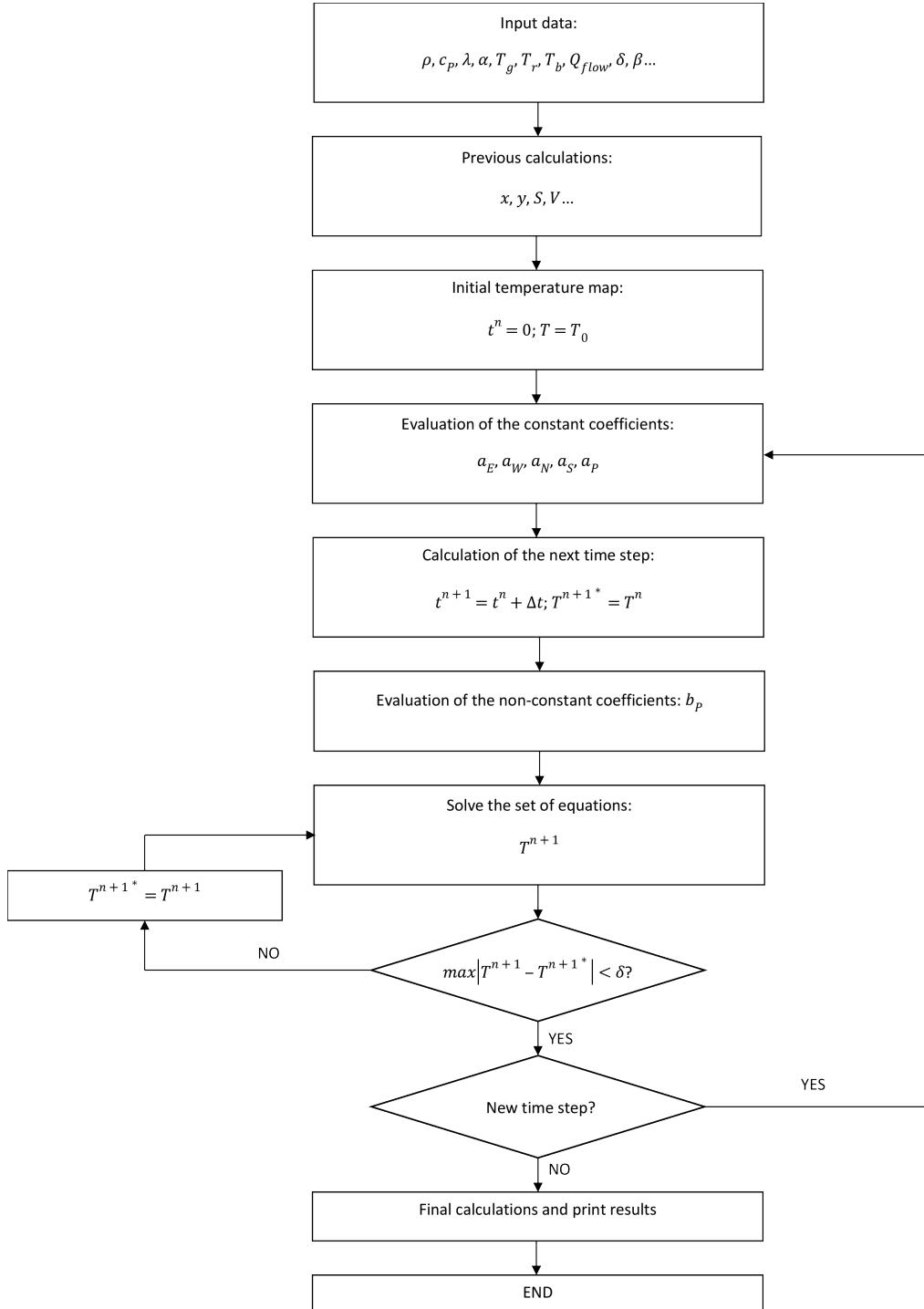
$$a_S = 0 \quad (4.9)$$

$$a_P = a_E + a_W + a_N + a_S + \frac{\rho_P V_P \bar{c}_P}{\Delta t} + \beta \frac{\lambda_P S_s}{d_{Ps}} \quad (4.10)$$

$$\begin{aligned} b_P &= \frac{\rho_P V_P \bar{c}_P T_P^n}{\Delta t} + \beta \left(\dot{q}_{vP}^{n+1} V_P + \frac{\lambda_P S_s}{d_{Ps}} T_b \right) \\ &+ (1 - \beta) \left[-\lambda_w \frac{T_P - T_W}{d_{PW}} S_w + \lambda_e \frac{T_E - T_P}{d_{PE}} S_e - \lambda_P \frac{T_P - T_b}{d_{Ps}} S_s + \lambda_n \frac{T_N - T_P}{d_{PN}} S_n + \dot{q}_{vP} V_P \right]^n \end{aligned} \quad (4.11)$$

4.3 Algorithm

The algorithm used in this convection problem is represented below. In this case, some of the discretization coefficients are constant, but sometimes they are not. These would change slightly the algorithm used.



4.4 Results

To verify the simulation, the results obtained are compared with some reference values for a time of 5000 s. As it can be seen in figures 4.2 and 4.2, the results of the code are very similar to the reference values.

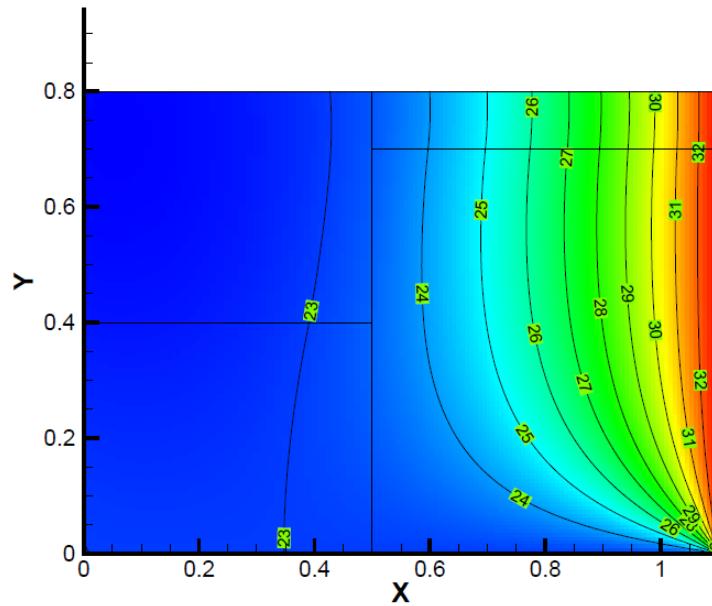


Figure 4.2: Reference value: Instantaneous isotherms at $t = 10000/2$ s

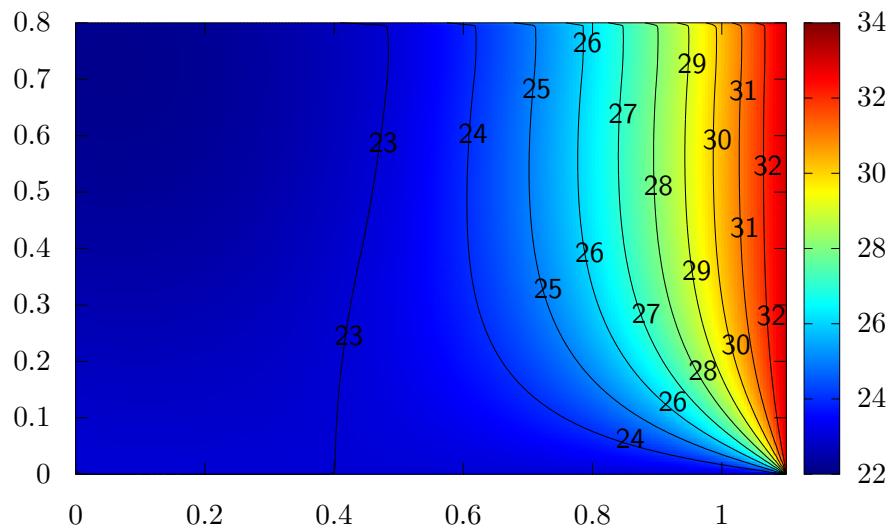


Figure 4.3: Instantaneous isotherm at $t=5000$ s

The four materials problem is transitory. Since the temperature in the right wall changes over time, it never reaches a steady state. To obtain some results, the final time of the simulation has been chosen to be 10000 s, as in the results of the figure 4.4.

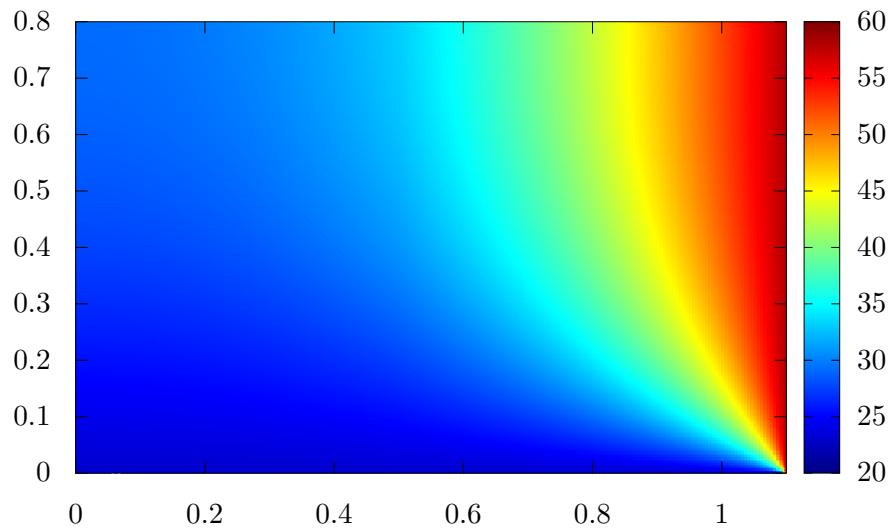


Figure 4.4: Instantaneous plot at $t=10000$ s

Nevertheless, to analyse the results obtained, the same simulation has been run for a homogeneous material (figure 4.5). The geometrical parameters and the boundary conditions have been maintained, but the physical properties of the whole material are those of the section M_2 of the four materials problem.

Comparing both graphs, it can be stated that the final result is very similar in both cases. The main visible difference is that in the four materials problem, the higher temperatures move further to the left. In the original problem, the upper right region is made of the material M_4 , which has the same conductivity as the homogeneous material M_2 , but a higher density and specific heat, making the first material more capable of conducting the heat.

Results

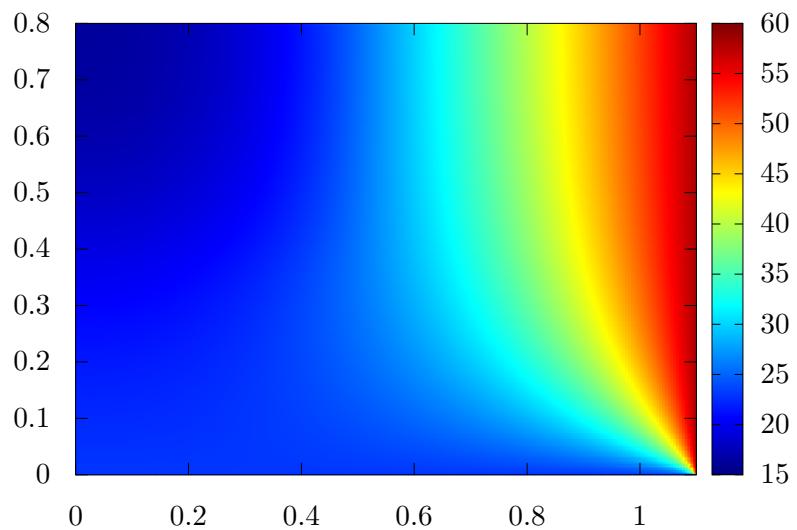


Figure 4.5: Instantaneous plot at $t=10000$ s for a homogeneous material

Part IV

Convection

5 | Convection

Convective heat transfer is the study of heat transport processes due to the flow of fluids [4]. Inside a fluid there may be different temperatures: some parts of it can have a higher temperature and others a lower temperature. The movement of liquids or gases combined with the temperature gradient causes convection [3].

This heat transfer occurs in the layers of a fluid, or can also occur between a solid and the fluid that is in contact with it. In both cases, the heat transfer depends on the properties of the fluid and its motion. As a consequence, to understand the heat transfer in a fluid or between a solid and a fluid, it is necessary to know the properties of the fluid itself.

5.1 The generic convection-diffusion equation

The motion of a fluid is described by the Navier-Stokes equations or conservation equations. As discussed in section 2.1, the Navier-Stokes equations are a particular case of the generic convection diffusion-equation 5.1:

$$\frac{\partial}{\partial t} (\rho\phi) + \nabla \cdot (\rho\vec{v}\phi) = \nabla \cdot (\Gamma\nabla\phi) + S_{phi} \quad (5.1)$$

where ρ is the density, \vec{v} the velocity, Γ the diffusion coefficient, S_ϕ the source term, and ϕ the general variable that is going to be studied. Some examples can be found in table 2.1.

5.2 Discretization

It is necessary to discretize equation 5.1 in space and time. The spatial discretization is done dividing the domain in different control volumes with a Cartesian grid. The node centred distribution is used, as specified in figure 5.1. The boundary nodes are in blue and the inner nodes in black.

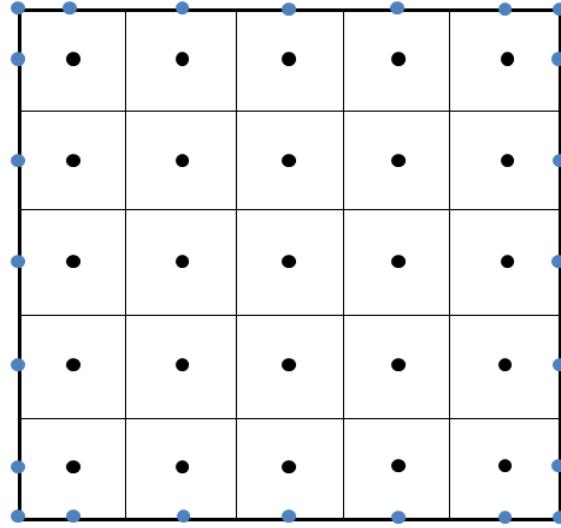


Figure 5.1: Mesh of the Smith-Hutton problem

To do so, it is easier to start with the discretization of the mass equation 5.2:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (5.2)$$

The first step is to integrate Equation 5.2 over time and space. Taking only the first term of the equation:

$$\int_{t^n}^{t^{n+1}} \int_{V_P} \frac{\partial \rho}{\partial t} dV dt = \int_{t^n}^{t^{n+1}} V_P \frac{\partial \bar{\rho}_P}{\partial t} dt = V_P (\bar{\rho}_P^{n+1} - \bar{\rho}_P^n) \approx V_P (\rho_P^{n+1} - \rho_P^n) = V_P (\rho_P - \rho_0) \quad (5.3)$$

Using the Divergence Theorem, the second term of the mass equation transforms into a surface integral. Then, to integrate over time, an implicit scheme is used.

$$\begin{aligned} \int_{t^n}^{t^{n+1}} \int_{V_P} \nabla \cdot (\rho \vec{v}) dV dt &= \int_{t^n}^{t^{n+1}} \int_{S_f} \rho \vec{v} \cdot \vec{n} dS dt = \\ &\int_{t^n}^{t^{n+1}} (\dot{m}_e - \dot{m}_w + \dot{m}_n - \dot{m}_s) dt \approx [\dot{m}_e - \dot{m}_w + \dot{m}_n - \dot{m}_s]^{n+1} \Delta t \end{aligned} \quad (5.4)$$

The final discretized mass equation is 5.5:

$$\frac{V_P (\rho_P - \rho_0)}{\Delta t} + \dot{m}_e - \dot{m}_w + \dot{m}_n - \dot{m}_s = 0 \quad (5.5)$$

The discretization of the convection-diffusion equation is very similar to that of the mass equation. Integrating over the volume the transport term of equation 5.1 and applying the Divergence Theorem:

$$\int_{V_P} \nabla \cdot (\rho \vec{v} \phi) = \int_{S_f} \rho \phi \vec{v} \cdot \vec{n} dS = \dot{m}_e \phi_e - \dot{m}_w \phi_w + \dot{m}_n \phi_n - \dot{m}_s \phi_s \quad (5.6)$$

The same procedure is used for the diffusion term of equation 5.1:

$$\int_{V_P} \nabla \cdot (\Gamma \nabla \phi) = \int_{S_f} \Gamma \cdot \nabla \phi \cdot \vec{n} dS = -\Gamma_w \frac{\partial \phi}{\partial x}|_w S_w + \Gamma_e \frac{\partial \phi}{\partial x}|_e S_e - \Gamma_s \frac{\partial \phi}{\partial x}|_s S_s + \Gamma_n \frac{\partial \phi}{\partial x}|_n S_n \approx D_e (\phi_E - \phi_P) - D_w (\phi_P - \phi_W) + D_n (\phi_N - \phi_P) - D_s (\phi_P - \phi_S) \quad (5.7)$$

where

$$D_e = \frac{\Gamma_e S_e}{d_{PE}} \quad (5.8)$$

$$D_w = \frac{\Gamma_w S_w}{d_{PW}} \quad (5.9)$$

$$D_n = \frac{\Gamma_n S_n}{d_{PN}} \quad (5.10)$$

$$D_s = \frac{\Gamma_s S_s}{d_{PS}} \quad (5.11)$$

To simplify the source term, it is linearized:

$$\int_{V_P} S_\phi dV \approx S_{\phi,P} V_P = (S_c^\phi + S_p^\phi \phi_P) V_P \quad (5.12)$$

So that the resulting discretized equation is:

$$\frac{\rho_P \phi_P - \rho_P^0 \phi_P^0}{\Delta t} V_P + \dot{m}_e \phi_e - \dot{m}_w \phi_w + \dot{m}_n \phi_n - \dot{m}_s \phi_s = D_e (\phi_E - \phi_P) - D_w (\phi_P - \phi_W) + D_n (\phi_N - \phi_P) - D_s (\phi_P - \phi_S) + S_{\phi,P} V_P \quad (5.13)$$

Multiplying by ϕ the discretized mass equation 5.5 and subtracting the result in 5.13, the discretized convection-diffusion equation is obtained:

$$\rho_P^0 \frac{\phi_P - \phi_P^0}{\Delta t} V_P + \dot{m}_e (\phi_e - \phi_P) - \dot{m}_w (\phi_w - \phi_P) + \dot{m}_n (\phi_n - \phi_P) - \dot{m}_s (\phi_s - \phi_P) = D_e (\phi_E - \phi_P) - D_w (\phi_P - \phi_W) + D_n (\phi_N - \phi_P) - D_s (\phi_P - \phi_S) + S_{\phi,P} V_P \quad (5.14)$$

The final step is to find an expression to evaluate the properties in the faces of the control volume, not in the nodes.

5.3 Evaluation of the value in the faces

To simplify the problem, a new variable is introduced to the problem: the total flux [2]. This variable is split in the two dimensions of the problem, the flux in the x-direction and the flux in the y-direction.

$$J_x \equiv \rho u \phi - \Gamma \frac{\partial \phi}{\partial x} \quad (5.15)$$

$$J_y \equiv \rho v \phi - \Gamma \frac{\partial \phi}{\partial y} \quad (5.16)$$

Introducing the expressions of the total flux 5.15 and 5.16 to equation 5.14, the discretized convection diffusion equation becomes:

$$\rho_P^0 \frac{\phi_P - \phi_P^0}{\Delta t} V_P + (J_e - F_e \phi_P) - (J_w - F_w \phi_P) + (J_n - F_n \phi_P) - (J_s - F_s \phi_P) = \\ \left(S_p^\phi \phi_P \right) V_P \quad (5.17)$$

where the flow rates are:

$$F_e = (\rho u)_e S_e \quad (5.18)$$

$$F_w = (\rho u)_w S_w \quad (5.19)$$

$$F_n = (\rho v)_n S_n \quad (5.20)$$

$$F_s = (\rho v)_s S_s \quad (5.21)$$

However, it is necessary to know how the fluxes are going to be evaluated. In order to use non-dimensional numbers, a new variable is defined:

$$J^* \equiv \frac{J\delta}{\Gamma} = P\phi - \frac{d\phi}{d(x/\delta)} \quad (5.22)$$

where P is the Péclet number and δ is the distance between the point that is going to be studied i , and the point next to it, $i + 1$. The value of ϕ and the value of the gradient $d\phi/d(x/\delta)$ are a combination of the ϕ_i and ϕ_{i+1} , so that J^* can be expressed as [2]:

$$J^* = B\phi_i - A\phi_{i+1} \quad (5.23)$$

The coefficients A and B are dimensionless and depend on the Péclet number. However, B is a combination of A and the Péclet number, and both coefficients are symmetric [2]. Taking these properties into account and introducing the operator $[A, B]$ that denotes the greater of A and B , it can be deduced that:

$$A(P) = A(|P|) + [-P, 0] \quad (5.24)$$

$$B(P) = A(|P|) + [-P, 0] \quad (5.25)$$

Introducing equations 5.24 and 5.25 into 5.17, the following formulation is obtained:

$$a_P \phi_P = a_E \phi_E + a_W \phi_W + a_N \phi_N + a_S \phi_S + b_P \quad (5.26)$$

where

$$a_E = D_e A(|P_e|) + [-F_e, 0] \quad (5.27)$$

$$a_W = D_w A(|P_w|) + [F_w, 0] \quad (5.28)$$

$$a_N = D_n A(|P_n|) + [-F_n, 0] \quad (5.29)$$

$$a_S = D_s A(|P_s|) + [-F_s, 0] \quad (5.30)$$

$$a_P = a_E + a_W + a_N + a_S + \frac{\rho_P^0 V_P}{\Delta t} - S_P V_P \quad (5.31)$$

$$b_P = S_c V_P + \frac{\rho_P^0 V_P}{\Delta t} \phi_P^0 \quad (5.32)$$

And the Péclet numbers are:

$$P_e = \frac{F_e}{D_e} \quad (5.33)$$

$$P_w = \frac{F_w}{D_w} \quad (5.34)$$

$$P_n = \frac{F_n}{D_n} \quad (5.35)$$

$$P_s = \frac{F_s}{D_s} \quad (5.36)$$

The only operation that should be defined is the value of the coefficient A . This value depends on the integration scheme that is going to be used. Some of its values are listed in table 5.1.

Scheme	Formula for $A(P_s)$
Central difference (CDS)	$1 - 0.5 P $
Upwind (UDS)	1
Hybrid (HDS)	$[0, 1 - 0.5 P]$
Power law (PLDS)	$[0, (1 - 0.5 P)^5]$
Exponential (EDS)	$ P / [\exp(P) - 1]$

Table 5.1: Function $A(|P|)$ for different schemes. Extracted from [2]

6 | Smith-Hutton problem

The Smith-Hutton problem is a two-dimensional steady convection-diffusion problem, represented in figure 6.1. In the problem, the density is constant, and the velocity field is known.

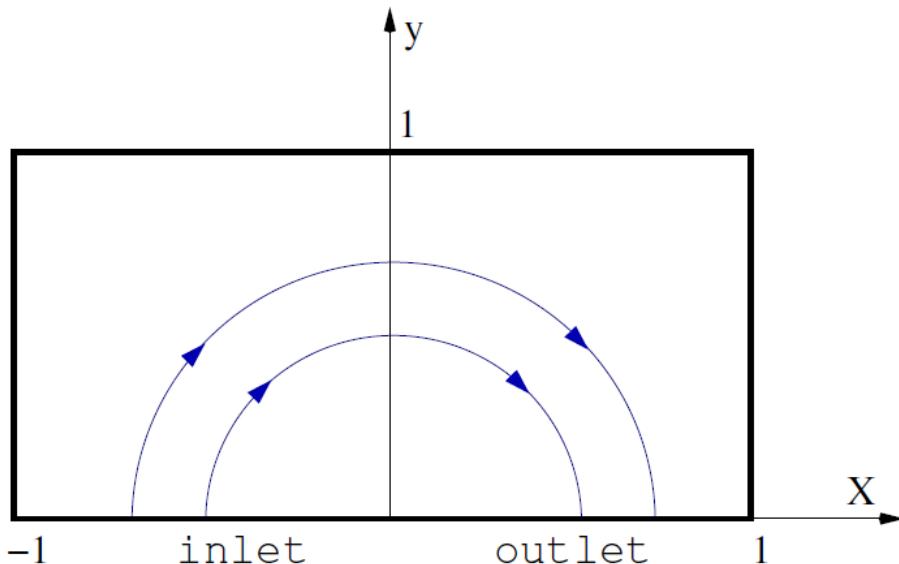


Figure 6.1: General scheme of the Smith-Hutton problem

The velocity is given by equations 6.1 and 6.2:

$$u(x, y) = 2y(1 - x^2) \quad (6.1)$$

$$v(x, y) = -2x(1 - y^2) \quad (6.2)$$

And the prescribed boundary conditions for the variable ϕ are described in equation 6.3:

$$\begin{aligned} \phi &= 1 + \tanh(\alpha(2x + 1)), & y = 0; x \in (-1, 0) & \text{(inlet)} \\ \frac{\partial \phi}{\partial y} &= 0, & x = 0; y \in (-1, 0) & \text{(outlet)} \\ \phi &= 1 - \tanh(\alpha), & \text{(elsewhere)} \end{aligned} \quad (6.3)$$

where $\alpha = 10$.

6.1 Discretization

The spatial discretization is the one explained in section 5.2, and the temporal scheme used is the implicit one, as explained in the same section.

N_x	N_y	δ	Source term
200	100	10^{-9}	0

Table 6.1: Numerical parameters of the Smith-Hutton problem

6.2 Boundary conditions

To apply the boundary conditions to the problem, some modifications on the coefficients defined by equation 5.26 have to be done. The easiest one is for the points in the left, top and right sides of the domain, in which the value of ϕ is defined.

In the bottom it is necessary to distinguish between the inlet and the outlet. A similar approach to that of the left, top and right side is used to determine the coefficients of the points in the inlet. However, in the outlet the only condition is that the derivative of ϕ in the vertical direction is equal to zero. The following reasoning leads to:

$$\frac{\partial \phi}{\partial y} \approx \frac{\phi_N - \phi_P}{\Delta y} = 0 \quad (6.4)$$

$$\phi_P = \phi_N \quad (6.5)$$

The implementation of the boundary conditions in the problem is done with the discretization coefficients listed in table 6.2.

Coefficients	Left, top and right	Inlet (bottom)	Outlet (bottom)
a_E	0	0	0
a_W	0	0	0
a_N	0	0	1
a_S	0	0	0
a_P	1	1	1
b_P	$1 - \tanh(\alpha)$	$1 + \tanh(\alpha(2x + 1))$	0

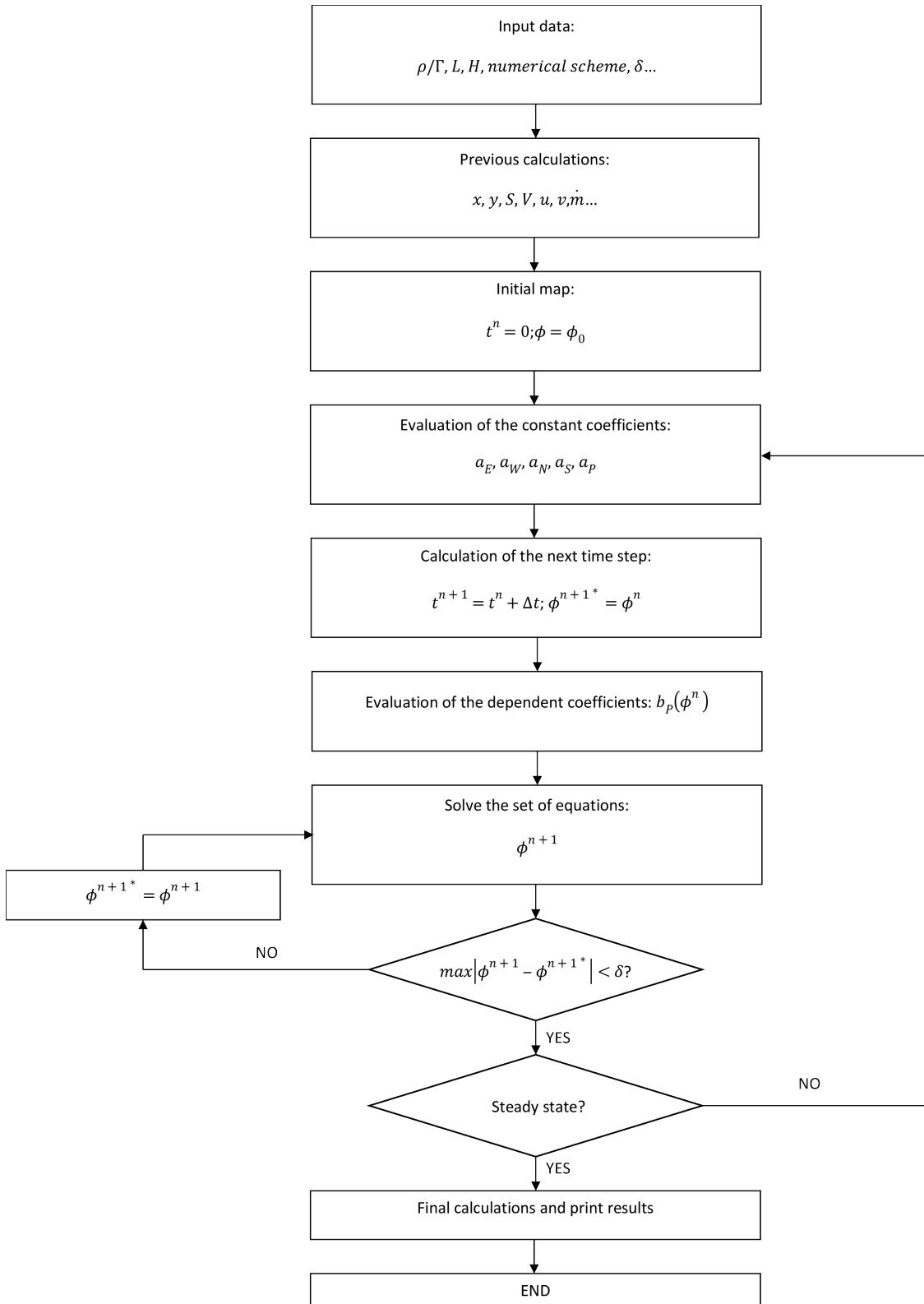
Table 6.2: Discretization coefficients of the boundary points

6.3 Algorithm

The algorithm of resolution is very similar to that used in the four materials problem. The main difference is that in the Smith-Hutton problem the resolution ends when the variable ϕ

Algorithm

reaches a steady state. The schematic resolution is displayed below:



6.4 Results

Some of the results are plotted in the following section, but due to the amount of information, not all of them are in the report. To see more results refer to Attachment A.

Since the velocity and the dimensions are constant, the parameter ρ/Γ is somehow equivalent to the Péclet number. In figure 6.2, when the Péclet number is low, all the methods have similar results, and there is almost no error compared to the reference values. However, as the Péclet number increases, the error increases, as it can be seen in figure 6.3 and figure 6.4.

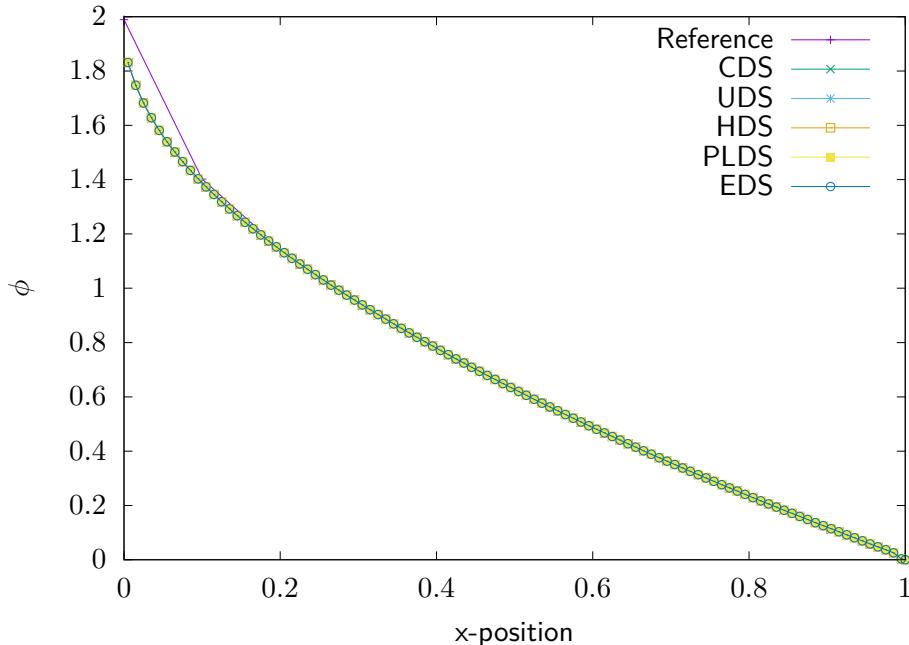


Figure 6.2: Comparative of the different methods $\rho/\Gamma = 10$

It is important to notice that in the cases in which $\rho/\Gamma = 10^3$ and $\rho/\Gamma = 10^6$ CDS diverges, and no results can be obtained with this method. It is not a surprise, because the central differencing scheme tends to diverge in some cases.

It is also important to understand the variation of the variable ϕ in the whole domain. For a low Péclet number (figure 6.5), the variation is very gradual. But as it increases (figures 6.6 and 6.7), the change is more abrupt, and there is almost no variation except for the centre bottom zone. The shape of the variation becomes more symmetrical as the Péclet number increases.

As a conclusion, it can be stated that when convergence dominates over diffusion (low Péclet numbers), velocity distributes the properties of the inlet to a great part of the domain. However, as diffusion becomes more important (the Péclet number increases), the influence of the inlet becomes less important.

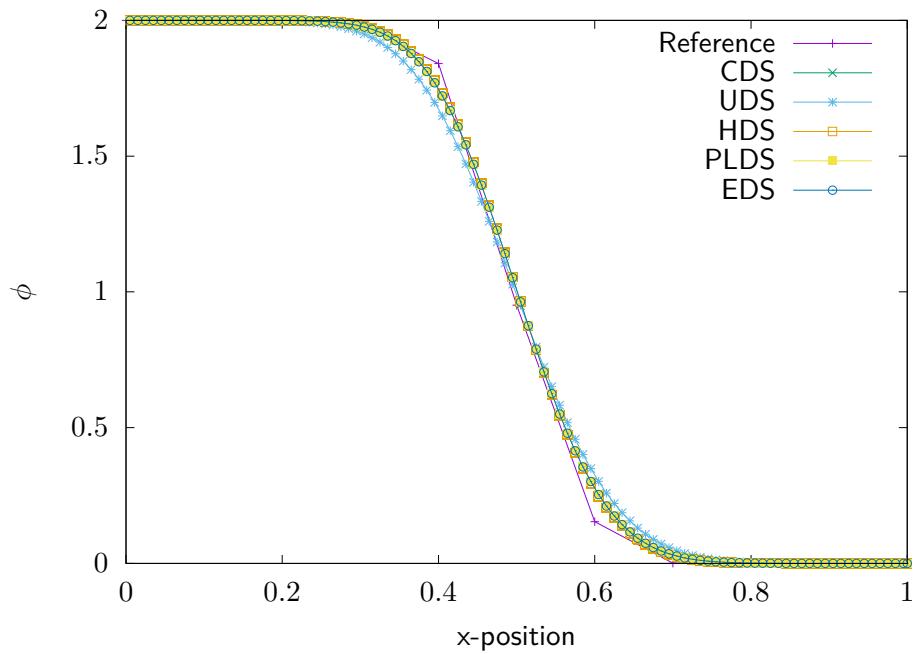


Figure 6.3: Comparative of the different methods $\rho/\Gamma = 10^3$

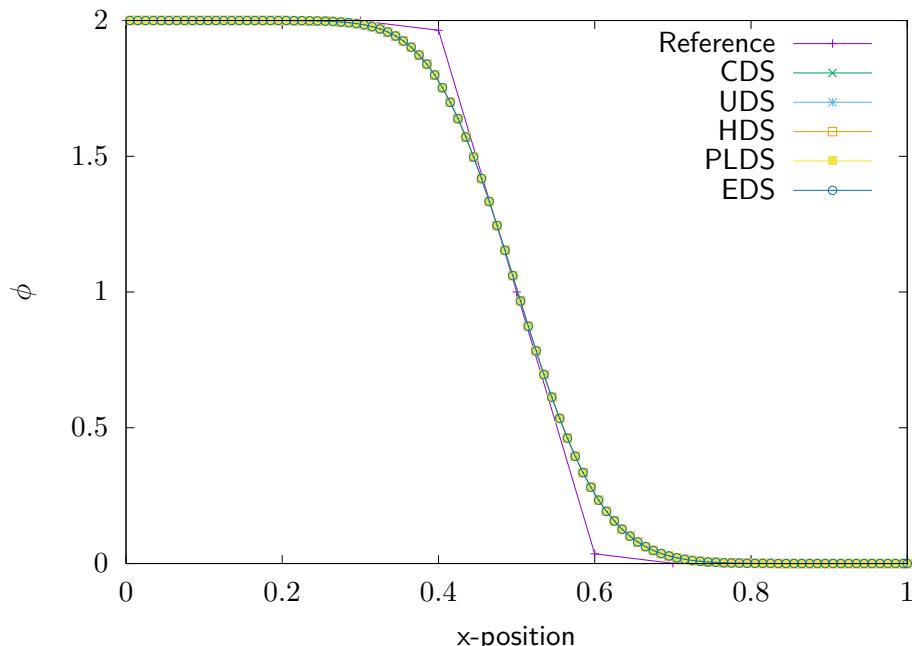


Figure 6.4: Comparative of the different methods $\rho/\Gamma = 10^6$

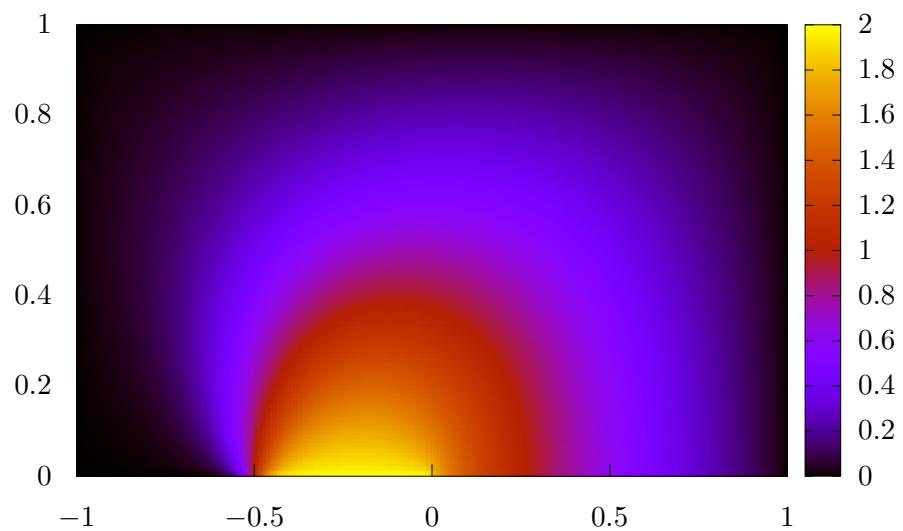


Figure 6.5: Representation of the whole domain for $\rho/\Gamma = 10$ (UDS)

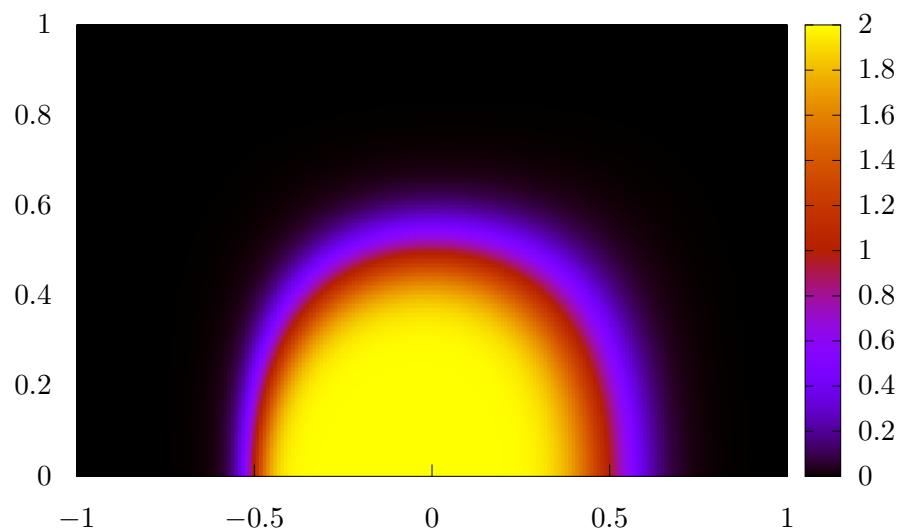


Figure 6.6: Representation of the whole domain for $\rho/\Gamma = 10^3$ (UDS)

Results

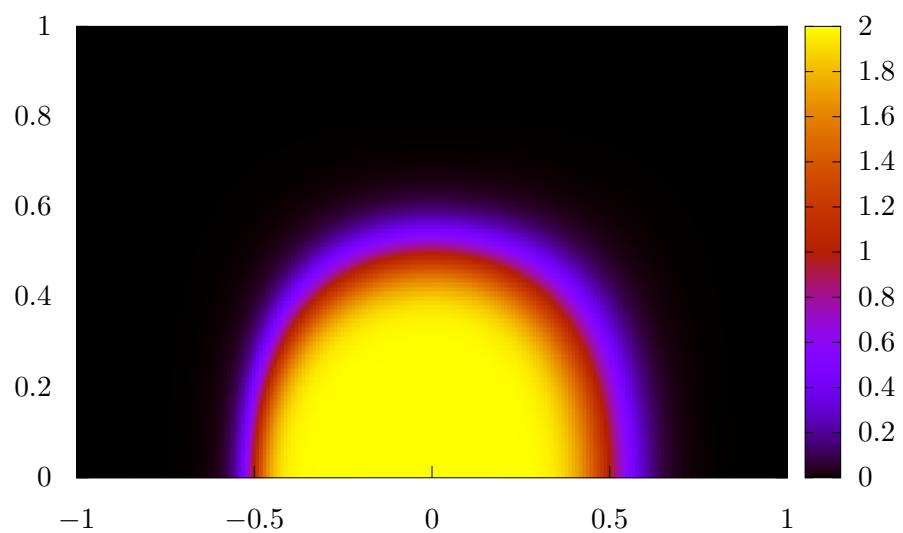


Figure 6.7: Representation of the whole domain for $\rho/\Gamma = 10^6$ (UDS)

7 | Fractional Step Method

The equations to be solved are the conservation of mass and the conservation of momentum:

$$\begin{aligned} \nabla \cdot \vec{v} &= 0 \\ \rho \frac{\partial \vec{v}}{\partial t} + \rho (\vec{v} \cdot \nabla) \vec{v} &= -\nabla p + \mu \nabla^2 \vec{v} \end{aligned} \quad (7.1)$$

According to the Helmholtz-Hodge theorem, it is possible to decompose any vector in a divergence-free vector parallel to the boundary and a gradient field, and this decomposition is unique [5].

Assuming constant density and viscosity, the convective and viscosity terms can be grouped together in a single variable $R(\vec{v})$, rewriting the Navier-Stokes equation as:

$$\rho \frac{\partial \vec{v}}{\partial t} = R(\vec{v}) - \nabla p \quad (7.2)$$

where $R(\vec{v}) = -\rho(\vec{v} \cdot \nabla) \vec{v} + \mu \nabla^2 \vec{v}$. Integrating the equation 7.2 over time:

$$\rho \frac{\vec{v}^{n+1} - \vec{v}^n}{\Delta t} = R^{n+\frac{1}{2}}(\vec{v}) - \nabla p^{n+1} \quad (7.3)$$

However, the term $R^{n+\frac{1}{2}}(\vec{v})$ is not easy to evaluate. To do so, the Adams-Bashforth second-order scheme is used:

$$R^{n+\frac{1}{2}}(\vec{v}) \approx \frac{3}{2}R(\vec{v}^n) - \frac{1}{2}R(\vec{v}^{n-1}) \quad (7.4)$$

Applying the Helmholtz-Hodge Theorem, the intermediate velocity is easily obtained:

$$\vec{v}^P = \vec{v}^{n+1} + \frac{\Delta t}{\rho} \nabla p^{n+1} \quad (7.5)$$

Introducing this expression to the integrated equation:

$$\rho \frac{\vec{v}^P - \vec{v}^n}{\Delta t} = R^{n+\frac{1}{2}}(\vec{v}) \quad (7.6)$$

And finally, applying the divergence to the expression of the intermediate velocity \vec{v}^P 7.5, the Poisson equation is obtained:

$$\nabla \cdot \vec{v} = \frac{\Delta t}{\rho} \nabla^2 p \quad (7.7)$$

7.1 Fractional Step Method algorithm

With all these expressions the fractional step method (FSM) can be finally implemented, following the next scheme:

1. Evaluate $R^{n+\frac{1}{2}}(\vec{v})$.
2. Calculate the intermediate velocity with equation 7.6.
3. Calculate the pressure p^{n+1} from the Poisson equation 7.7 using a linear solver.
4. Calculate the velocity at the next time step with equation 7.5.

However, the FSM can be problematic if the mesh of the problem is not correctly implemented. To avoid having solutions with no physical sense, it is important to use staggered meshes or collocated meshes. The discretization of the domain as well as a further explanation of the described steps are going to be developed in the following sections.

7.2 Discretization

To avoid convergence problems or incorrect solutions (checkerboard problem), the staggered meshes are used. As shown in figure 7.1, in a two-dimensional case there are 3 control volumes, one for each variable: p_P , u_P and v_P . They are coloured in black, red and green respectively. The black dots are the nodes in which the pressure is calculated, the red arrows are the nodes of the horizontal velocity, and the green arrows are the nodes of the vertical velocity.

7.2.1 Intermediate velocity discretization

First of all, it is necessary to discretize the expression of R of the equation 7.2:

$$R(\vec{v}) = -\rho(\vec{v} \cdot \nabla)\vec{v} + \mu\nabla^2\vec{v} \quad (7.8)$$

This variable is a vector. Integrating the expression over the control volume of the horizontal velocity staggered mesh in the horizontal direction:

$$\int_{\Omega_x} R(u) d\Omega_x = - \int_{\Omega_x} (\rho\vec{v} \cdot \nabla) u d\Omega_x + \int_{\Omega_x} \mu\nabla^2 u d\Omega_x \quad (7.9)$$

Now, applying the Gauss Theorem:

$$R(u) V_P = - \int_{\partial\Omega_x} (\rho\vec{v}) u \cdot \vec{n} dS + \int_{\partial\Omega_x} \mu\nabla u \cdot \vec{n} dS \quad (7.10)$$

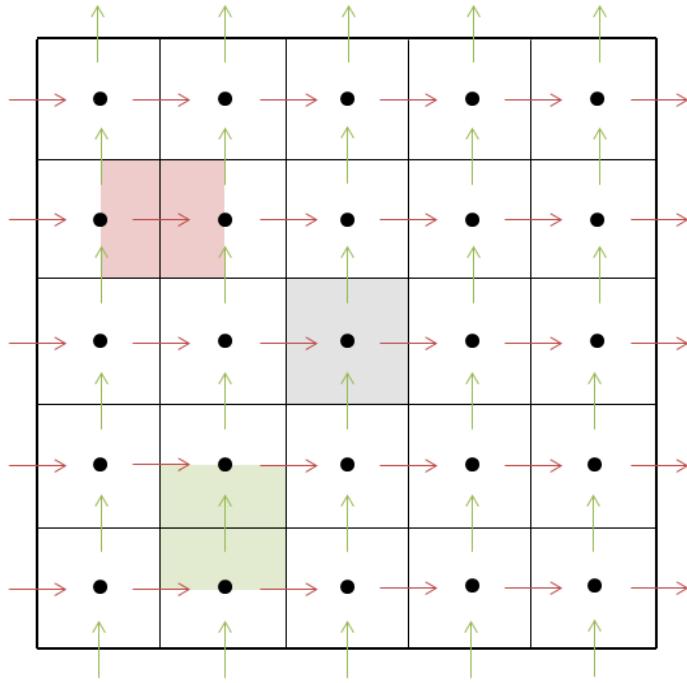


Figure 7.1: Staggered meshes (2D)

The final integration of R in the horizontal direction results as:

$$R(u) V_P = \left[\mu_e \frac{u_E - u_P}{d_{EP}} A_e + \mu_n \frac{u_N - u_P}{d_{NP}} A_n - \mu_w \frac{u_P - u_W}{d_{WP}} A_w - \mu_s \frac{u_P - u_S}{d_{SP}} A_s \right] - [(\rho u)_e u_e A_e + (\rho v)_n u_n A_n - (\rho u)_w u_w A_w - (\rho v)_s u_s A_s] \quad (7.11)$$

The same approach is used in the vertical direction, obtaining the following expression:

$$R(v) V_P = \left[\mu_e \frac{v_E - v_P}{d_{EP}} A_e + \mu_n \frac{v_N - v_P}{d_{NP}} A_n - \mu_w \frac{v_P - v_W}{d_{WP}} A_w - \mu_s \frac{v_P - v_S}{d_{SP}} A_s \right] - [(\rho u)_e v_e A_e + (\rho v)_n v_n A_n - (\rho u)_w v_w A_w - (\rho v)_s v_s A_s] \quad (7.12)$$

The main problem of these expressions is the evaluation of the velocities and the mass flows in the faces of the control volume. To calculate the velocities in the faces some of the numerical schemes previously discussed are used: CDS, UDS... In the case of the mass flows per surface unit, the staggered meshes have to be taken into account:

- The calculation of the mass flow per surface unit in the control volume of the horizontal velocity 7.2 is simple in the case of the horizontal mass flows:

$$(\rho u)_e = \frac{\rho u_P + \rho u_2}{2} \quad (7.13)$$

$$(\rho u)_w = \frac{\rho u_1 + \rho u_P}{2} \quad (7.14)$$

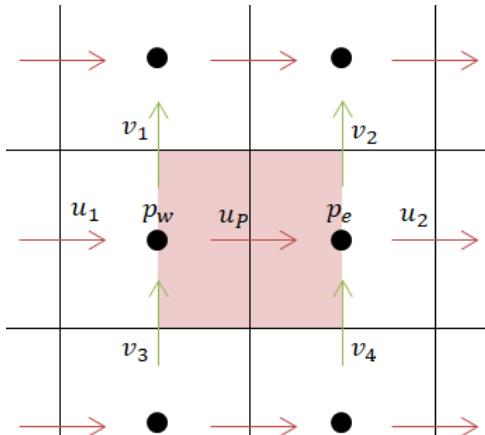


Figure 7.2: Control volume of the horizontal velocity

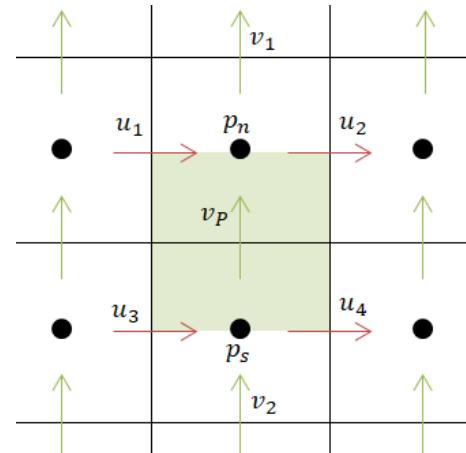


Figure 7.3: Control volume of the vertical velocity

But the vertical flows are somehow more difficult:

$$(\rho v)_n = \frac{\rho v_1 + \rho v_2}{2} \quad (7.15)$$

$$(\rho v)_s = \frac{\rho v_3 + \rho v_4}{2} \quad (7.16)$$

- The calculation of the mass flow per surface unit in the control volume of the vertical velocity 7.3 is similar to that of the horizontal velocity. Starting with the horizontal flows:

$$(\rho u)_e = \frac{\rho u_2 + \rho u_4}{2} \quad (7.17)$$

$$(\rho u)_w = \frac{\rho u_1 + \rho u_3}{2} \quad (7.18)$$

And the vertical ones:

$$(\rho v)_n = \frac{\rho v_1 + \rho v_P}{2} \quad (7.19)$$

$$(\rho v)_s = \frac{\rho v_P + \rho v_2}{2} \quad (7.20)$$

Once the value of R is calculated using the expressions developed above and the Adams-Bashforth scheme 7.4, the intermediate velocity can be computed rearranging the equation 7.6:

$$\vec{v}^P = \vec{v}^n + \frac{\Delta t}{\rho} R^{n+\frac{1}{2}} (\vec{v}) \quad (7.21)$$

7.2.2 Pressure discretization

The next step is to obtain the pressure in the next time step with the Poisson equation. Knowing the space discretization of the domain, the discretized Poisson equation can be

calculated. Integrating the expression 7.7 over the domain and applying the divergence theorem, the following expression can be easily obtained:

$$\frac{p_E^{n+1} - p_P^{n+1}}{d_{EP}} A_e + \frac{p_N^{n+1} - p_P^{n+1}}{d_{NP}} A_n - \frac{p_P^{n+1} - p_W^{n+1}}{d_{WP}} A_w - \frac{p_P^{n+1} - p_S^{n+1}}{d_{SP}} A_s = \frac{1}{\Delta t} [(\rho u^P)_e A_e + (\rho v^P)_n A_n - (\rho u^P)_w A_w - (\rho v^P)_s A_s] \quad (7.22)$$

Rewriting the equation using discretization coefficients:

$$a_P p_P^{n+1} = a_E p_E^{n+1} + a_W p_W^{n+1} + a_N p_N^{n+1} + a_S p_S^{n+1} + b_P \quad (7.23)$$

where

$$a_P = a_E + a_W + a_N + a_S \quad (7.24)$$

$$a_E = \frac{A_e}{d_{EP}} \quad (7.25)$$

$$a_W = \frac{A_w}{d_{WP}} \quad (7.26)$$

$$a_N = \frac{A_n}{d_{NP}} \quad (7.27)$$

$$a_S = \frac{A_s}{d_{SP}} \quad (7.28)$$

$$b_P = -\frac{1}{\Delta t} [(\rho u^P)_e A_e + (\rho v^P)_n A_n - (\rho u^P)_w A_w - (\rho v^P)_s A_s] \quad (7.29)$$

7.2.3 Velocity discretization

With the equation 7.5 the horizontal and vertical velocities at the next time step can be calculated:

$$u_P^{n+1} = u_P^n - \frac{\Delta t}{\rho} \frac{p_e^{n+1} - p_w^{n+1}}{d_{ew}} \quad (7.30)$$

$$v_P^{n+1} = v_P^n - \frac{\Delta t}{\rho} \frac{p_n^{n+1} - p_s^{n+1}}{d_{ns}} \quad (7.31)$$

7.3 Time step

The fractional step method is an explicit method. In order to obtain accuracy in the results, the time step has to be correctly chosen. To do so, it is recalculated in each iteration of the algorithm using a Courant-Friedrich-Levy (CFL) condition. Two time steps are defined, one of them depends on the convective term and the other one on the diffusive term:

$$\Delta t_c = \min \left(0.35 \frac{\Delta x}{|v|} \right) \quad (7.32)$$

$$\Delta t_d = \min \left(0.20 \frac{\rho (\Delta x)^2}{\mu} \right) \quad (7.33)$$

If the mesh, the density and the viscosity are constant, the time step defined by the diffusive term is constant, so it only has to be calculated at the beginning of the simulation, as it depends on the velocity. But the time step given by the convective term changes with each iteration. The final time step that is going to be used is the smallest one:

$$\Delta t = \min (\Delta t_c, \Delta t_d) \quad (7.34)$$

8 | Driven cavity problem

The driven cavity problem consists in a two-dimensional cavity with an incompressible fluid. The upper wall of the cavity moves at a given velocity, as shown in figure 8.1. The aim of the problem is to obtain the distribution of velocities inside the cavity.

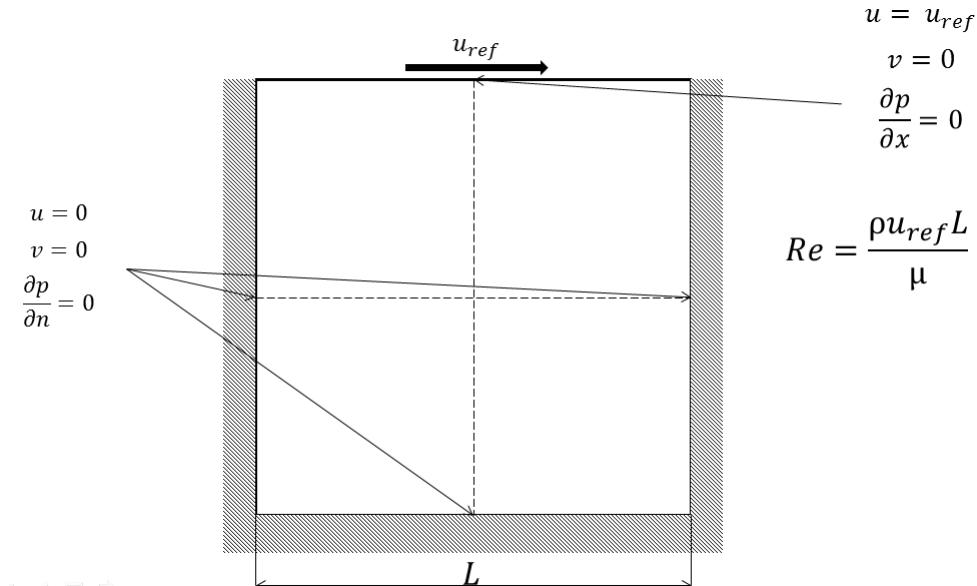


Figure 8.1: General scheme of the driven cavity problem. Extracted from [6]

8.1 Discretization

The domain is discretized, as explained in section 7.2, using the staggered meshes. To do so, the volume is divided using a Cartesian grid, with the following characteristics:

N	M	L	ρ	u_{ref}	μ	δ
100	100	1	1	1	$\frac{1}{Re}$	10^{-5}

Table 8.1: Numerical parameters of the driven cavity problem

The length of the cavity L , the density ρ , the velocity u_{ref} and the viscosity μ are chosen in order to have a non-dimensional problem.

8.2 Boundary conditions

It is necessary to impose the conditions defined by figure 8.1. There are two types of conditions: the prescribed velocity, and the boundary layer conditions. The last ones are defined by assuming that the pressure gradient normal to the wall is 0. For example, in the left wall:

$$\frac{\partial p}{\partial x} \approx \frac{p_E - p_P}{\Delta x} = 0 \quad (8.1)$$

$$p_P = p_E \quad (8.2)$$

These boundary layer conditions modify the discretization coefficients in the boundary nodes. The coefficients are listed in table 8.2.

Coefficients	Top	Bottom	Left	Right
a_E	1	0	1	0
a_W	0	0	0	1
a_N	0	1	0	0
a_S	0	0	0	0
a_P	1	1	1	1

Table 8.2: Discretization coefficients in the boundary

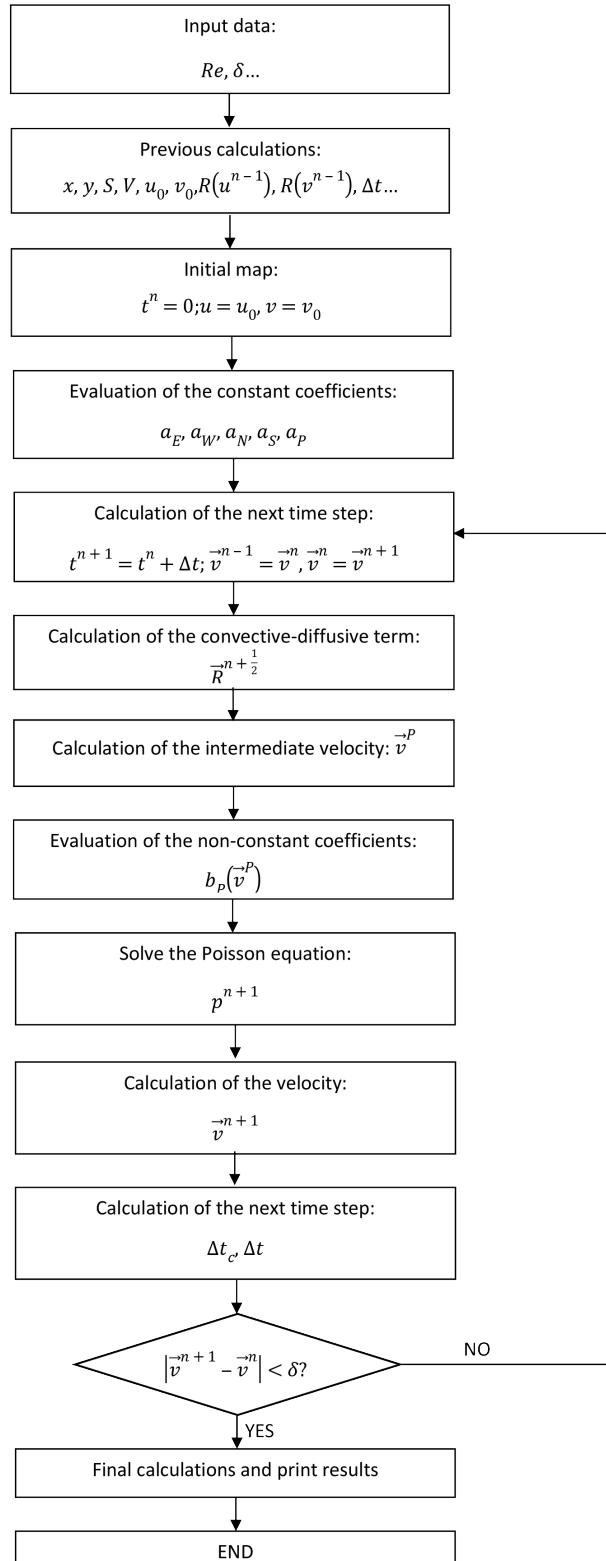
The condition of prescribed velocity in the walls is achieved with the following conditions:

- $R(\vec{v}) = 0$ in the top
- $R(\vec{v}) = 0$ in the bottom wall
- $R(\vec{v}) = 0$ in the left wall
- $R(\vec{v}) = 0$ in the right wall

And the prescribed velocities are:

- $u = u_{ref}, v = 0$ in the top
- $u = 0, v = 0$ in the bottom wall
- $u = 0, v = 0$ in the left wall
- $u = 0, v = 0$ in the right wall

8.3 Algorithm



The simulation of the driven cavity problem ends when it reaches a steady state.

8.4 Results

9 | Differentially heated cavity

The differentially heated cavity problem or buoyancy-driven cavity problem is a two dimensional problem based on free convection. It comprises a cavity with the vertical walls at different temperatures and adiabatic horizontal walls [7,8]. The difference of temperatures between the two vertical walls causes convection.

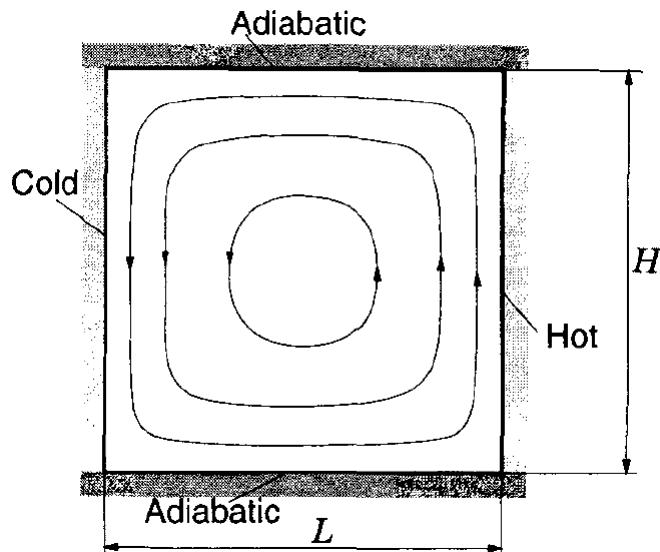


Figure 9.1: General scheme of the differentially heated problem. Extracted from [1]

9.1 Natural convection

The equations that are going to be discretized are the two-dimensional equations of mass, momentum and energy for a Newtonian fluid with constant properties. However, some approximations have to be done for the momentum equation:

$$\rho_0 \frac{\partial \vec{v}}{\partial t} + \rho_0 (\vec{v} \cdot \nabla) \vec{v} = -\nabla p + \mu \nabla^2 \vec{v} + \rho \vec{g} \quad (9.1)$$

As it can be seen, mass forces have been added to the momentum equation, because in natural convection gravity is not negligible. Another important remark is that the fluid is considered

incompressible, but this approximation is not applied in the gravitational term, because it is this term that causes the flow. However, as a simplification, the Boussinesq approximation is applied [3, 9]:

$$\rho = \rho_0 (1 - \beta (T - T_0)) \quad (9.2)$$

where β is the volumetric thermal expansion coefficient, a thermodynamic property that measures the variation of the density as a function of the temperature at a constant pressure. Introducing the Boussinesq approximation in the momentum equation, the final equations for natural convection are:

$$\nabla \cdot \vec{v} = 0 \quad (9.3)$$

$$\rho_0 \frac{\partial \vec{v}}{\partial t} + \rho_0 (\vec{v} \cdot \nabla) \vec{v} = -\nabla p_d + \mu \nabla^2 \vec{v} - \rho_0 \beta (T - T_0) \vec{g} \quad (9.4)$$

$$\rho c_p \left(\frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T \right) = \lambda \nabla^2 T \quad (9.5)$$

9.1.1 Non-dimensional equations

In order to have a simpler analysis, it is convenient to use non-dimensional variables. Depending on the problem, they can be defined by several different ways. In this section, taking into account the most important variables of a free convection problem, the dimensionless variables are defined as it is expressed below:

$$\vec{x}^* = \frac{\vec{x}}{L} \quad (9.6)$$

$$\vec{v}^* = \frac{\vec{v}}{\frac{\lambda}{\rho L c_P}} \quad (9.7)$$

$$t^* = \frac{t}{\frac{\rho L^2 c_P}{\lambda}} \quad (9.8)$$

$$p^* = \frac{p}{\frac{1}{\rho} \left(\frac{\lambda}{c_P L} \right)^2} \quad (9.9)$$

$$T^* = \frac{T - T_{cold}}{T_{hot} - T_{cold}} \quad (9.10)$$

Inserting these expressions in the equations 9.3, 9.4 and 9.5, the non-dimensional equations for natural convection are obtained. In order to simplify the notation, the indexes * have been removed, but the variables that are represented in the following section are the dimensionless ones.

$$\nabla \cdot \vec{v} = 0 \quad (9.11)$$

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v} = -\nabla p + Pr \nabla^2 \vec{v} - Pr Ra T \vec{u}_g \quad (9.12)$$

$$\frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T = \nabla^2 T \quad (9.13)$$

The dimensionless numbers that appear are the Prandtl and Rayleigh numbers, defined as:

$$Pr \equiv \frac{c_P \mu}{\lambda} \quad (9.14)$$

$$Ra \equiv \frac{\rho^2 g \beta \Delta T L^3 c_P}{\mu \lambda} \quad (9.15)$$

where $\Delta T = T_{hot} - T_{cold}$.

9.2 Application of the fractional step method

The resolution of this problem can be done using the fractional step method described in chapter 7. In the case of the momentum equation its resolution is done as it is explained in the mentioned section. But the expression of the equation is slightly different. Rewriting the momentum equation as it was done:

$$\frac{\partial \vec{v}}{\partial t} = R(\vec{v}) - \nabla p \quad (9.16)$$

where

$$R(\vec{v}) = -(\vec{v} \cdot \nabla) \vec{v} + Pr \nabla^2 \vec{v} - Pr Ra T \vec{u}_g \quad (9.17)$$

The other important issue is the introduction of the energy equation. It has to be discretized according to the fractional step method. As it can be seen, this case is very similar to the previously studied Smith-Hutton problem, since the velocity field is "known" (calculated by other means) and the unknown is a scalar. Therefore, an implicit scheme is going to be used for the temporal integration:

$$\frac{T^{n+1} - T^n}{\Delta t} = [-\vec{v} \cdot \nabla T + \nabla^2 T]^{n+1} \quad (9.18)$$

9.3 Discretization

The spatial discretization of the domain is the one described by the figure 7.1: a Cartesian grid with a staggered mesh.

The discretization of the momentum equation is very similar to that described in the fractional step method chapter but adding the gravity term in the case of the vertical equation:

$$R(u) V_P = \left[Pr_e \frac{u_E - u_P}{d_{EP}} A_e + Pr_n \frac{u_N - u_P}{d_{NP}} A_n - Pr_w \frac{u_P - u_W}{d_{WP}} A_w - Pr_s \frac{u_P - u_S}{d_{SP}} A_s \right] \\ - [(u)_e u_e A_e + (v)_n u_n A_n - (u)_w u_w A_w - (v)_s u_s A_s] \quad (9.19)$$

Boundary conditions

$$R(v) V_P = \left[Pr_e \frac{v_E - v_P}{d_{EP}} A_e + Pr_n \frac{v_N - v_P}{d_{NP}} A_n - Pr_w \frac{v_P - v_W}{d_{WP}} A_w - Pr_s \frac{v_P - v_S}{d_{SP}} A_s \right] - [(u)_e v_e A_e + (v)_n v_n A_n - (u)_w v_w A_w - (v)_s v_s A_s] - Pr Ra T V_P \quad (9.20)$$

In the case of the energy equation a similar approach is used. Temperature, like pressure, is evaluated in the nodes, not in the faces like the velocities. The integration of the terms of the equations starts with the Gauss Theorem:

$$\int_{\Omega} \vec{v} \nabla T d\Omega = \int_{\partial\Omega} \vec{v} \cdot \vec{n} T dS \approx (u)_e T_e A_e + (v)_n T_n A_n - (u)_w T_w A_w - (v)_s T_s A_s \quad (9.21)$$

$$\int_{\Omega} \nabla^2 T d\Omega = \int_{\partial\Omega} \nabla T dS \approx \frac{T_E - T_P}{d_{PE}} A_e + \frac{T_N - T_P}{d_{PN}} A_n - \frac{T_P - T_W}{d_{PW}} A_w - \frac{T_P - T_S}{d_{PS}} A_s \quad (9.22)$$

The temperature in the faces is evaluated using the central differencing scheme, as it was done for the velocities.

The final discretized equation for the temperature can be expressed as:

$$a_P T_P = a_E T_E + a_W T_W + a_N T_N + a_S T_S + b_p \quad (9.23)$$

where the discretized coefficients are the same discussed in the section 5.3.

9.4 Boundary conditions

Since the cavity is all surrounded by walls, the boundary velocities are:

- $\vec{v} = 0$ in the top wall
- $\vec{v} = 0$ in the bottom wall
- $\vec{v} = 0$ in the left wall
- $\vec{v} = 0$ in the right wall

In the case of the temperature, they are determined in the right and left walls. Taking into account the expression of T in the equation 9.10:

- $T = 0$ in the left wall
- $T = 1$ in the right wall

In the top and bottom walls the only condition is that they are adiabatic. This condition can also be expressed as:

$$\frac{\partial T}{\partial y} \approx \frac{T_P - T_S}{d_{PS}} = 0 \quad (9.24)$$

$$T_P = T_S \quad (9.25)$$

As a consequence, the discretized coefficients of the boundary nodes have the values listed in table 9.1.

Coefficients	Left	Right	Top	Bottom
a_E	0	0	0	0
a_W	0	0	0	0
a_N	0	0	0	1
a_S	0	0	1	0
a_P	1	1	1	1
b_P	0	1	0	0

Table 9.1: Discretization coefficients of the boundary temperature nodes

9.5 Nusselt number

In the differentially heated cavity, the motion occurs due to the convective transfer. In other words, the temperature gradient is the important issue in this problem, so it would be useful to calculate it. The local heat flux in a horizontal direction at any point in the cavity [8]:

$$Q(x, y) = uT - \frac{\partial T}{\partial x} \quad (9.26)$$

The Nusselt number is a non-dimensional parameter that can be seen as the dimensionless temperature gradient. It provides a measure of the convection heat at a surface [3]. The local Nusselt number gives the heat flow through any vertical line:

$$Nu_x = \int_0^1 Q(x, y) dy \quad (9.27)$$

Another useful value is the average Nusselt number of the whole cavity:

$$\bar{Nu} = \int_0^1 Nu_x dx \quad (9.28)$$

Part V

Turbulence

10 | Burgers' equation

Burgers' equation, also known as Burgulence, is a one dimensional approach to the Navier-Stokes equations in an incompressible flow. Taking the dimensionless expressions that describe an incompressible flow:

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v} = \frac{1}{Re} \nabla^2 \vec{v} - \nabla p \quad (10.1)$$

$$\nabla \cdot \vec{v} = 0 \quad (10.2)$$

And writing their one-dimensional form, the Burgers equation is easily obtained:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \frac{1}{Re} \frac{\partial^2 u}{\partial x^2} + f \quad (10.3)$$

where u is the velocity in the studied dimension and f the source term.

Since the equation is one-dimensional, the continuity equation 10.2 is removed. The pressure gradient is also removed because it depends on the continuity equation.

10.1 Fourier space

The easiest way to solve the equation is to solve it in Fourier space. The basic approach of this space is that any function can be represented as a sum of sinus and cosines known as Fourier series in the following way:

$$u(x) = \sum_{k=-\infty}^{k=+\infty} \hat{u}_k e^{ikx} \quad (10.4)$$

where $e^{ikx} = \cos(kx) + i \sin(kx)$.

Nonetheless, in a numerical calculation, it is impossible to have an infinite number of terms, it is necessary to have a finite number. This is not a problem, because in spectral methods, the biggest amount of information is in the lowest frequencies, which means that it is not

necessary to have a huge amount of terms in order to have a proper solution of the equation. Taking this into account, the functions that are represented in the Fourier space become a sum of a finite number of sinus and cosines:

$$u(x) = \sum_{k=-N}^{k=+N} \hat{u}_k e^{ikx} \quad (10.5)$$

Using this expression, the Burgers' equation can be transformed into the Fourier space. However, the derivatives have to be calculated. Applying the derivative to the Fourier function definition:

$$\frac{\partial u}{\partial x} = \frac{\partial}{\partial x} \sum_{k=-N}^{k=+N} \hat{u}_k e^{ikx} = \sum_{k=-N}^{k=+N} \hat{u}_k \frac{\partial e^{ikx}}{\partial x} = \sum_{k=-N}^{k=+N} \hat{u}_k (ik) e^{ikx} \quad (10.6)$$

The same procedure is applied to the second derivative in order to obtain the diffusive term:

$$\begin{aligned} \frac{\partial^2 u}{\partial x^2} &= \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} \right) = \frac{\partial}{\partial x} \sum_{k=-N}^{k=+N} \hat{u}_k (ik) e^{ikx} = \sum_{k=-N}^{k=+N} \hat{u}_k (ik) \frac{\partial e^{ikx}}{\partial x} = \\ &\quad \sum_{k=-N}^{k=+N} \hat{u}_k (ik)^2 e^{ikx} = \sum_{k=-N}^{k=+N} (-k^2 \hat{u}_k) e^{ikx} \end{aligned} \quad (10.7)$$

The transient 10.8 and forcing 10.9 terms are straightforward:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial t} \sum_{k=-N}^{k=+N} \hat{u}_k e^{ikx} \quad (10.8)$$

$$f = \sum_{k=-N}^{k=+N} F_k e^{ikx} \quad (10.9)$$

On the other, the convective term is more complicated. This non-linear term is a multiplication of the function u and its derivative, and when this term is transformed into Fourier space there are some things that need to be taken into account. The terms in question are:

$$\frac{\partial u}{\partial x} = \sum_{q=-N}^{q=+N} iq \hat{u}_q e^{iqx} \quad (10.10)$$

$$u = \sum_{p=-N}^{p=+N} \hat{u}_p e^{ipx} \quad (10.11)$$

As it is noted, the variable k has been renamed in both terms in order to avoid confusions when the expressions are multiplied to obtain the convective term. It is finally calculated as:

$$u \frac{\partial u}{\partial x} = \sum_{p,q} \hat{u}_p iq \hat{u}_q e^{i(p+q)x} \quad (10.12)$$

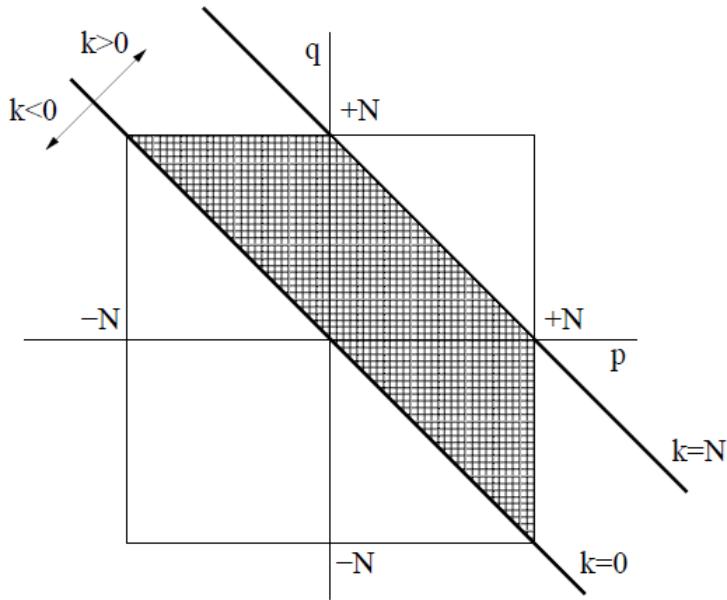


Figure 10.1: Representation of all the possible interactions between the modes in the convective term. Extracted from [10]

Taking all these expressions, integrating them into the Burgers equation and applying the Fourier transform, the final expression is:

$$\frac{\partial \hat{u}_k}{\partial t} + \sum_{p+q=k} \hat{u}_p i q \hat{u}_q = -\frac{k^2}{Re} \hat{u}_k + F_k \quad (10.13)$$

for $k = 1, \dots, N$; and where $\hat{u}_k \in \mathbb{C}$.

As it can be seen, one of the main advantages of spectral methods is that all the modes can be solved separately. However, due to the convective term, there is still a sum of terms in the equation, which can be named triadic interactions. This summation can be easily interpreted with figure 10.1. In Fourier space $\hat{u}_{-k} = \hat{u}_k$, so only the positive modes need to be solved. Moreover, since the Fourier series are truncated for $k \leq |N|$, the only possible interactions are those of $p + q \leq N$. Therefore, only the interactions between the lines $k = 0$ and $k = +N$ have to be considered in the computation of the convective term.

10.2 Discretization

In order to solve the equation it is necessary to discretize it over time. The time-integration scheme used is the fully explicit one:

$$\frac{\hat{u}_k^{n+1} - \hat{u}_k^n}{\Delta t} + \sum_{p+q=k} \hat{u}_q i q \hat{u}_q = -\frac{k^2}{Re} \hat{u}_k + F_k \quad (10.14)$$

However, the time step needs to be small enough to guarantee good results. A CFL-like condition is imposed:

$$\Delta t \leq C_1 \frac{Re}{N^2} \quad (10.15)$$

10.2.1 Large-Eddy Simulation

The method proposed in the previous lines is called Direct Numerical Simulation (DNS), and it does not provide as good results as other methods based on some turbulence models. A method that can improve the calculations is the Large-Eddy Simulation (LES). Like the DNS, it starts with a one-dimensional equation in which the unknown is not the velocity but its average.

$$\frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} = \frac{1}{Re} \frac{\partial^2 \bar{u}}{\partial x^2} + f - \frac{\partial}{\partial x} \tau(u) \quad (10.16)$$

where

$$\tau(u) = \bar{u}^2 - \bar{u}^2 \quad (10.17)$$

In the Smagorinsky model, this subfilter tensor is modeled using a viscosity called the eddy-viscosity:

$$\tau(u) \approx \nu_t \frac{\partial \bar{u}}{\partial x} \quad (10.18)$$

Smagorinsky also obtained an expression for ν_t , but it cannot be applied in Fourier space. To do so, a spectral viscosity model is used:

$$\nu_t(k/k_N) = \nu_t^{+\infty} \left(\frac{E_{k_N}}{k_N} \right)^{1/2} \nu_t^* \left(\frac{k}{k_N} \right) \quad (10.19)$$

where

$$\nu_t^{+\infty} = 0.31 \frac{5-m}{m+1} \sqrt{3-m} C_K^{-3/2} \quad (10.20)$$

$$\nu_t^* \left(\frac{k}{k_N} \right) = 1 + 34.5 e^{-3.03(k_N/k)} \quad (10.21)$$

where m is the slope of the energy spectrum, E_{k_N} is the energy at the truncated frequency k_N , and C_K is the Kolmogorov constant. With the results obtained with the DNS, it can be deduced that $m = 2$ approximately. And for the value of the Kolomogorov constant, it is known that for the one-dimensional Burgers' equation it is $C_K \approx 0.4523$.

10.3 Results

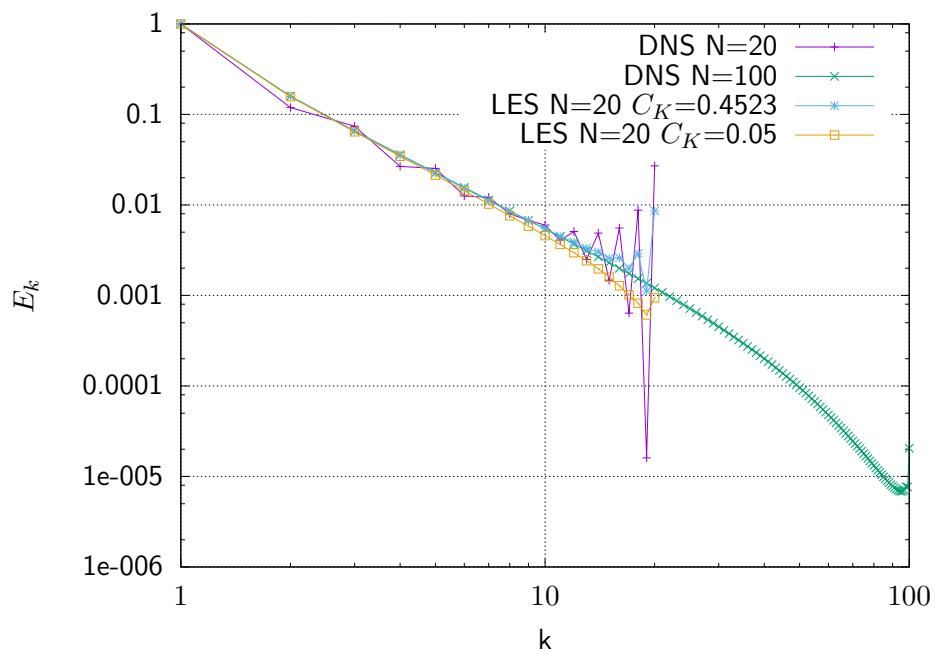


Figure 10.2: Energy spectrum of the steady-state solution of the Burgers' equation

11 | Bibliography

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