UNIVERSITAT POLITÈCNICA DE CATALUNYA
BARCELONATECH
Escola Superior d'Enginyeries Industrial,
Aeroespacial i Audiovisual de Terrassa

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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

**Author:** Laura Pla Olea
**Director:** Carlos David Perez Segarra
**Co-Director:** Asensio Oliva Llena
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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 Advantatges 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:

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

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

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

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

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

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

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

where $\rho$ is the density, $\vec{v}$ the velocity, $\Gamma$ the diffusion coefficient, $S_\phi$ the source term, and $\phi$ the general variable that is going to be studied. Some examples can be found in table 2.1.

| Equation | $\phi$ | $\Gamma$ | $S_\phi$ |
|---|---|---|---|
| Mass conservation | $1$ | $0$ | $0$ |
| Momentum | $\vec{v}$ | $\mu$ | $-\nabla p + \nabla \cdot \vec{\tau} + \rho\vec{g} + \vec{f^e}$ |
| Energy (for a semiperfect gas) | $u$ | $\lambda/c_v$ | $-\nabla \cdot \vec{q} - p\nabla \cdot \vec{v} + \vec{\tau} : \nabla\vec{v} + \Phi^e$ |

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 $\phi$ of a grid point only influences the distribution of $\phi$ 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:

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

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

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

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

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

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.

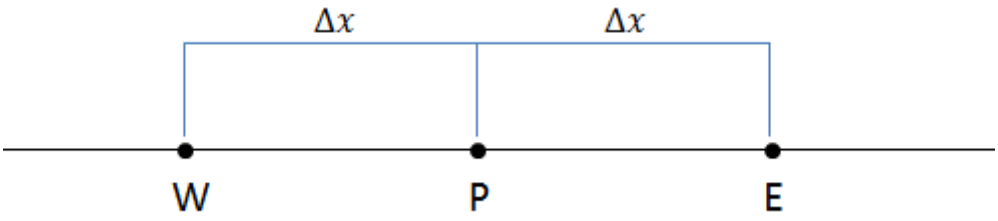



Figure 2.1: Three successive grid points

## 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.

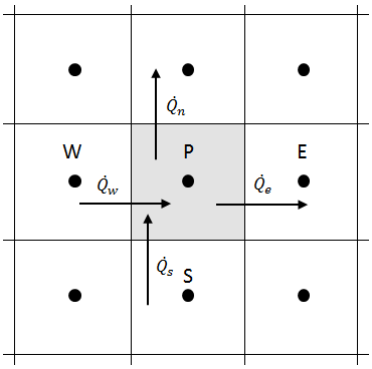



Figure 2.2: Control volume (2D)

### 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:

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

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 $\phi$ in the interface is equal to the value of $\phi$ at the node on the upwind side of the face.

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

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 $\Gamma$ 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 $\phi_0$ and $\phi_L$ 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 is described by equation 3.1:

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

Where $\rho$ is the density of the material, $T$ the temperature, $\lambda$ 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:

$$\vec{q} = -\lambda \frac{\partial T}{\partial n} \vec{n} \tag{3.2}$$

## 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.

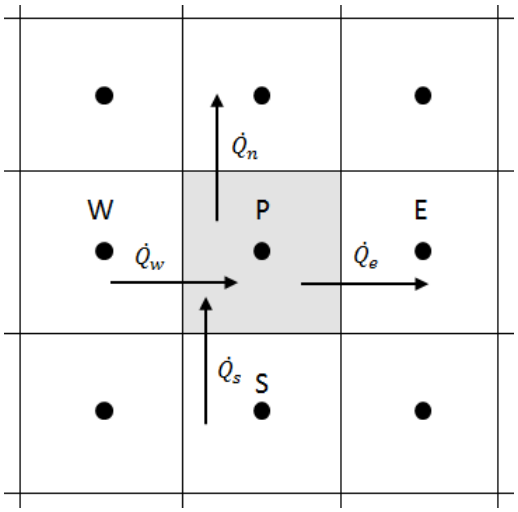



Figure 3.1: Heat fluxes through the faces of a control volume

### 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.

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

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

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

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

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

The inner heat of the material can be discretized as:

$$Q_{VP} = \int_{V_P} \dot{q}_v dV \approx \dot{q}_{vP} V_P \tag{3.7}$$

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:

$$\dot{q}_e^- = \dot{q}_e^+ \tag{3.8}$$

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

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

$$\lambda_e = \frac{d_{PE}}{\frac{d_{Pe}}{\lambda_P} + \frac{d_{Ee}}{\lambda_E}} \tag{3.11}$$

### 3.2.2 Temporal discretization

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

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

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:

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

Rearranging the first term of the equation:

$$\int_{t^n}^{t^{n+1}} \rho_P \frac{\partial \bar{u}_P}{\partial t} V_P dt = \rho_P V_P \left(\bar{u}_P^{n+1} - \bar{u}_P^n\right) \approx \rho_P V_P \left(u_P^{n+1} - u_P^n\right) = \rho_P V_P \bar{c}_P \left(T_P^{n+1} - T_P^n\right) \tag{3.14}$$

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

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

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

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

where

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

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

$$a_P T_P = a_E T_E + a_W T_W + a_N T_N + a_S T_S + b_P \tag{3.18}$$

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

$$a_E = \beta \frac{\lambda_e S_e}{d_{PE}} \tag{3.19}$$

$$a_W = \beta \frac{\lambda_w S_w}{d_{PW}} \tag{3.20}$$

$$a_N = \beta \frac{\lambda_n S_n}{d_{PN}} \tag{3.21}$$

$$a_S = \beta \frac{\lambda_s S_s}{d_{PS}} \tag{3.22}$$

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

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

## 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.

$$T_{wall} = T_{prescribed} \tag{3.25}$$

- 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.

$$\dot{q}_{wall} = \dot{q}_{prescribed} \tag{3.26}$$

- 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:

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

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

$$\dot{q}_{conduction} = \dot{q}_{convection} \tag{3.29}$$

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

where $T_g$ is the temperature of the fluid next to the wall, $\alpha$ 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.

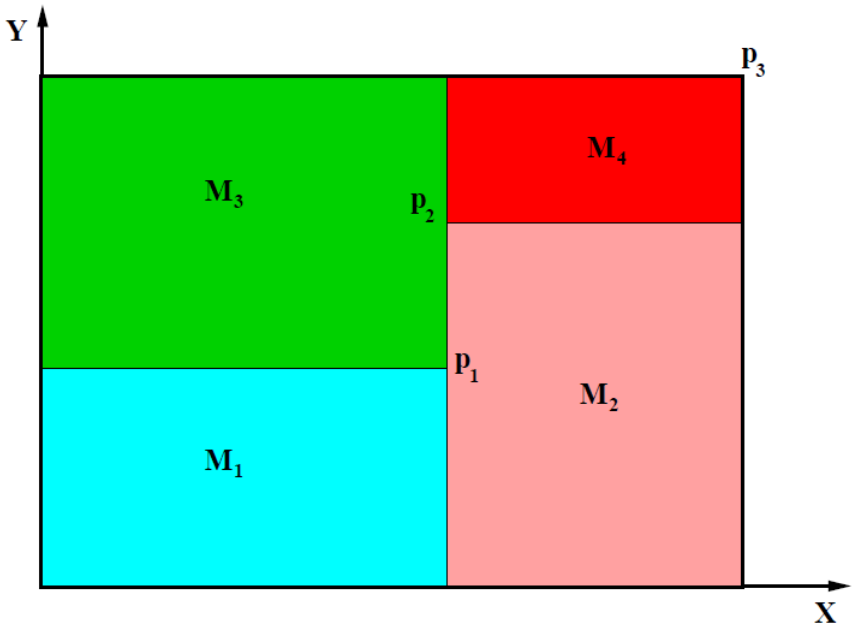



Figure 4.1: General scheme of the four materials problem

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

Table 4.3: Boundary conditions

The initial temperature field is $T = 8.00°C$.

## 4.1 Discretization

The spatial discretization of the problem is that described in section 3.2.1, and the temporal discretization the one described in section 3.2.2.

## 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:

$$a_W = 0 \tag{4.1}$$

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

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

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:

$$a_N = 0 \tag{4.4}$$

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

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:

$$a_E = 0 \tag{4.6}$$

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

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

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:

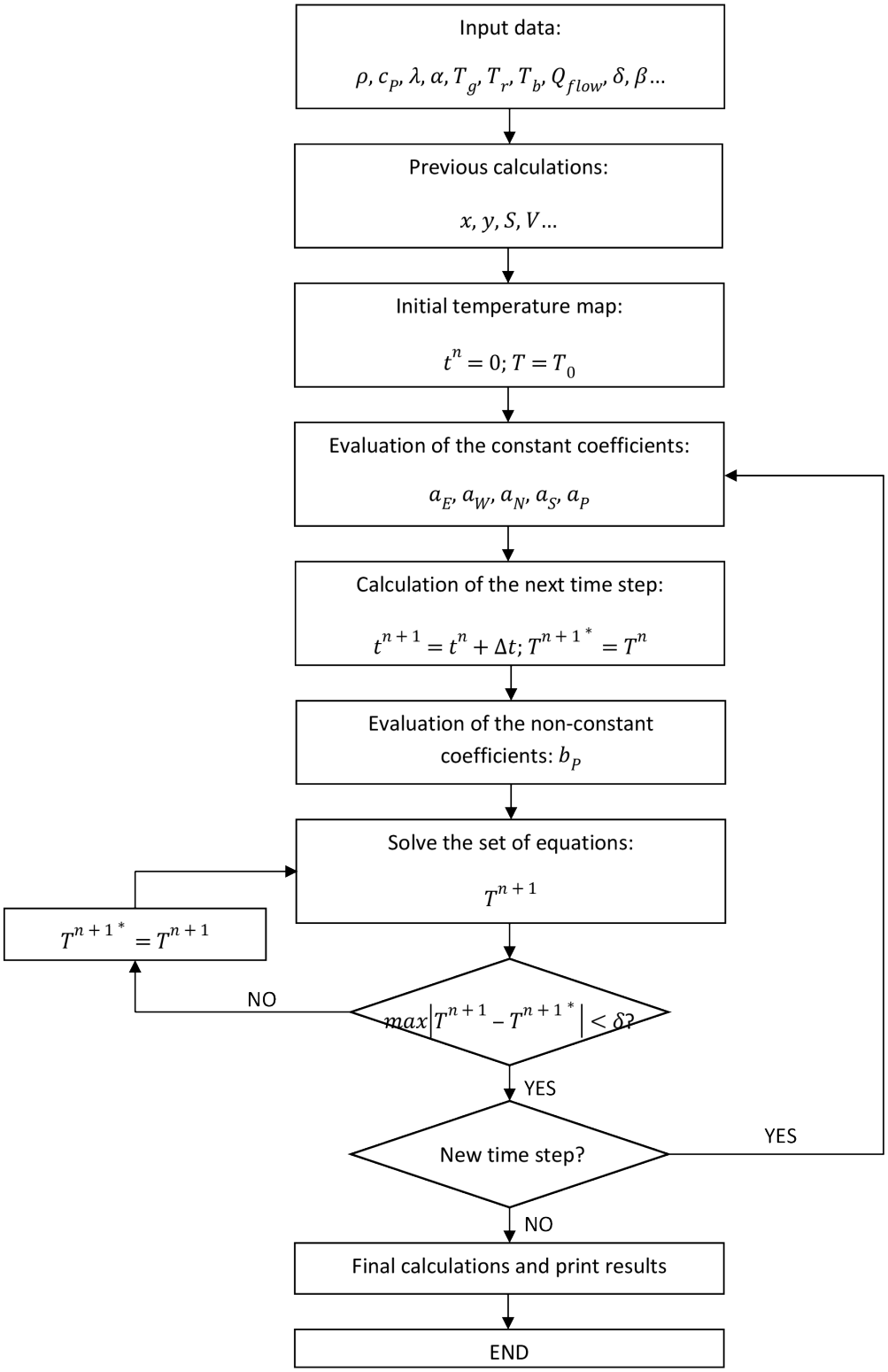
$$a_S = 0 \tag{4.9}$$

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

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

## 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.


Input data:
$\rho, c_P, \lambda, \alpha, T_g, T_r, T_b, Q_{flow}, \delta, \beta \ldots$
Previous calculations:
$x, y, S, V \ldots$
Initial temperature map:
$t^n = 0; T = T_0$
Evaluation of the constant coefficients:
$a_E, a_W, a_N, a_S, a_P$
Calculation of the next time step:
$t^{n+1} = t^n + \Delta t; T^{n+1\,*} = T^n$
Evaluation of the non-constant coefficients: $b_P$
Solve the set of equations:
$T^{n+1}$
$T^{n+1\,*} = T^{n+1}$
NO
$max\left|T^{n+1} - T^{n+1\,*}\right| < \delta$?
YES
New time step?
YES
NO
Final calculations and print results
END

## 4.4 Results

# Part IV

# Convection

# 5 | The Navier-Stokes Equations

The mathematical formulation needed to solve this problem is the convection diffusion-equation 5.1:

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

# 6 | Smith-Hutton problem

The Smith-Hutton problem is a two-dimensional steady convection-diffusion problem, represented in figure 6.1. In this problem, the density is constant, and the velocity field is known. The velocity field is given by equations 6.1 and 6.2:

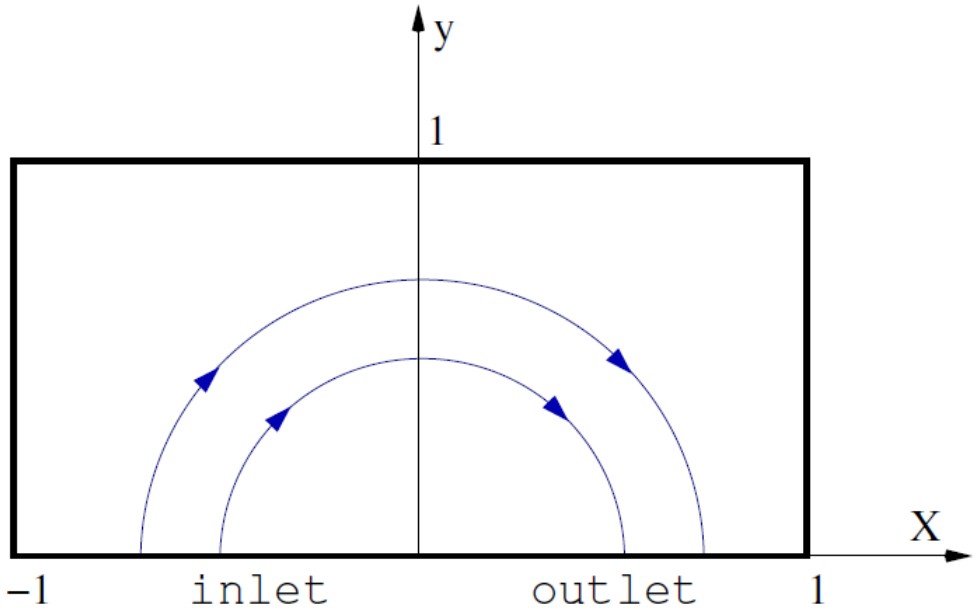



Figure 6.1: General scheme of the Smith-Hutton problem

$$u\left(x,y\right)=2y\left(1-x^{2}\right) \tag{6.1}$$

$$v\left(x,y\right)=-2x\left(1-y^{2}\right) \tag{6.2}$$

And the prescribed boundary conditions for the variable $\phi$ are described in equation 6.3:

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

where $\alpha=10$.

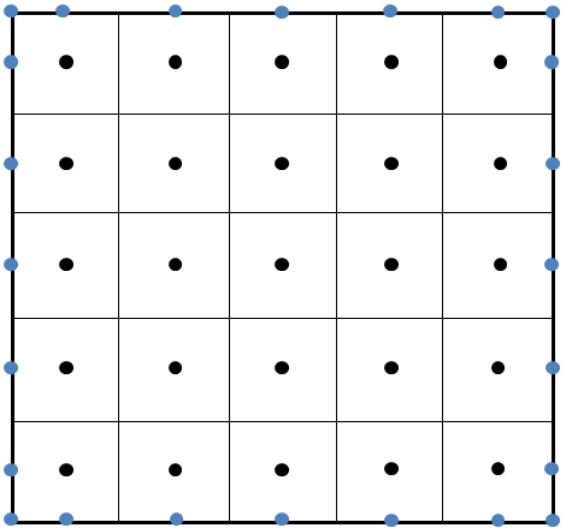


Figure 6.2: Mesh of the Smith-Hutton problem

## 6.1 Discretization

It is necessary to discretize equation 5.1 in space and time. The control volume used to discretize the problem is specified in figure 6.2. The boundary nodes are in blue and the inner nodes in black. To do so, it is easier to start with the discretization of the mass equation 6.4:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \tag{6.4}$$

The first step is to integrate Equation 6.4 over time and space. Taking only the first term of the equation:

$$\begin{aligned} \int_{t^n}^{t^{n+1}} \int_{V_P} \frac{\partial \rho}{\partial t} dV dt = \int_{t^n}^{t^{n+1}} V_P \frac{\partial \bar{\rho}_P}{\partial t} dt = V_P \left( \bar{\rho}_P^{n+1} - \bar{\rho}_P^n \right) \approx \\ V_P \left( \rho_P^{n+1} - \rho_P^n \right) = V_P \left( \rho_P - \rho_0 \right) \end{aligned} \tag{6.5}$$

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.

$$\int_{t^n}^{t^{n+1}} \int_{V_P} \nabla \cdot (\rho \vec{v}) \, dV dt = \int_{t^n}^{t^{n+1}} \int_{S_f} \rho \vec{v} \cdot \vec{n} dS dt =$$

$$\int_{t^n}^{t^{n+1}} \left( \dot{m}_e - dotm_w + dotm_n - dotm_s \right) dt \approx \left[ \dot{m}_e - dotm_w + dotm_n - dotm_s \right]^{n+1} \Delta t \tag{6.6}$$

The final discretized mass equation is 6.7:

$$\frac{V_P \left( \rho_P - \rho_0 \right)}{\Delta t} + \dot{m}_e - dotm_w + dotm_n - dotm_s = 0 \tag{6.7}$$

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:

$$\int_{V_P} \nabla \cdot (\rho \vec{v} \phi) = \int_{S_f} \rho \phi \vec{v} \cdot \vec{n} dS = \dot{m}_e \phi_e - \dot{m}_w \phi_w + \dot{m}_n \phi_n - \dot{m}_s \phi_s \tag{6.8}$$

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

$$\int_{V_P} \nabla \cdot (\Gamma \nabla \phi) = \int_{S_f} \Gamma \cdot \nabla \phi \cdot \vec{n} dS = -\Gamma_w \frac{\partial \phi}{\partial x}\Big|_w S_w + \Gamma_e \frac{\partial \phi}{\partial x}\Big|_e S_e - \Gamma_s \frac{\partial \phi}{\partial x}\Big|_s S_s + \Gamma_n \frac{\partial \phi}{\partial x}\Big|_n S_n \approx$$
$$D_e (\phi_E - \phi_P) - D_w (\phi_P - \phi_W) + D_n (\phi_N - \phi_P) - D_s (\phi_P - \phi_S) \Big| \tag{6.9}$$

where

$$D_e = \frac{\Gamma_e S_e}{d_{PE}} \tag{6.10}$$

$$D_w = \frac{\Gamma_w S_w}{d_{PW}} \tag{6.11}$$

$$D_n = \frac{\Gamma_n S_n}{d_{PN}} \tag{6.12}$$

$$D_s = \frac{\Gamma_s S_s}{d_{PS}} \tag{6.13}$$

To simplify the source term, it is linearized:

$$\int_{V_P} S_\phi dV \approx S_{\phi,P} V_P = \left(S_c^\phi + S_p^\phi \phi_P\right) V_P \tag{6.14}$$

So that the resulting discretized equation is:

$$\frac{\rho_P \phi_P - \rho_P^0 \phi_P^0}{\Delta t} V_P + \dot{m}_e \phi_e - \dot{m}_w \phi_w + \dot{m}_n \phi_n - \dot{m}_s \phi_s =$$
$$D_e (\phi_E - \phi_P) - D_w (\phi_P - \phi_W) + D_n (\phi_N - \phi_P) - D_s (\phi_P - \phi_S) + S_{\phi,P} V_P \tag{6.15}$$

Multiplying by $\phi$ the discretized mass equation 6.7 and subtracting the result in 6.15, the discretized convection-diffusion equation is obtained:

$$\rho_P^0 \frac{\phi_P - \phi_P^0}{\Delta t} V_P + \dot{m}_e (\phi_e - \phi_P) - \dot{m}_w (\phi_w - \phi_P) + \dot{m}_n (\phi_n - \phi_P) - \dot{m}_s (\phi_s - \phi_P) = D_e (\phi_E - \phi_P) - D_w (\phi_P - \phi_W \tag{6.16}$$

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

$$J_x \equiv \rho u \phi - \Gamma \frac{\partial \phi}{\partial x} \tag{6.17}$$

$$J_y \equiv \rho v \phi - \Gamma \frac{\partial \phi}{\partial y} \tag{6.18}$$

Introducing the expressions of the total flux 6.17 and 6.18 to 6.16, the discretized convection diffusion equation becomes:

$$\rho_P^0 \frac{\phi_P - \phi_P^0}{\Delta t} V_P + (J_e - F_e \phi_P) - (J_w - F_w \phi_P) + (J_n - F_n \phi_P) - (J_s - F_s \phi_P) = \left(S_p^\phi \phi_P\right) V_P \tag{6.19}$$

where the flow rates are:

$$F_e = (\rho u)_e S_e \tag{6.20}$$

$$F_w = (\rho u)_w S_w \tag{6.21}$$

$$F_n = (\rho v)_n S_n \tag{6.22}$$

$$F_s = (\rho v)_s S_s \tag{6.23}$$

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:

$$J^* \equiv \frac{J\delta}{\Gamma} = P\phi - \frac{d\phi}{d\,(x/\delta)} \tag{6.24}$$

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

$$J^* = B\phi_i - A\phi_{i+1} \tag{6.25}$$

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:

$$A\,(P) = A\,(|P|) + [-P, 0] \tag{6.26}$$

$$B\,(P) = A\,(|P|) + [-P, 0] \tag{6.27}$$

Introducing equations 6.26 and 6.27 into 6.19, the following formulation is obtained:

$$a_P\phi_P = a_E\phi_E + a_W\phi_W + a_N\phi_N + a_S\phi_S + b_P \tag{6.28}$$

where

$$a_E = D_e A\,(|P_e|) + [-F_e, 0] \tag{6.29}$$

$$a_W = D_w A\,(|P_w|) + [F_w, 0] \tag{6.30}$$

$$a_N = D_n A\,(|P_n|) + [-F_n, 0] \tag{6.31}$$

$$a_S = D_s A\,(|P_s|) + [-F_s, 0] \tag{6.32}$$

$$a_P = a_E + a_W + a_N + a_S + \frac{\rho_P^0 V_P}{\Delta t} - S_P V_P \tag{6.33}$$

$$b_P = S_c V_P + \frac{\rho_P^0 V_P}{\Delta t}\phi_P^0 \tag{6.34}$$

And the Péclet numbers are:

$$P_e = \frac{F_e}{D_e} \tag{6.35}$$

| 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 6.1: Function $A(|P|)$ for different schemes [?]

$$P_w = \frac{F_w}{D_w} \tag{6.36}$$

$$P_n = \frac{F_n}{D_n} \tag{6.37}$$

$$P_s = \frac{F_s}{D_s} \tag{6.38}$$

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 6.1.

# 7 | Fractional Step Method

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

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

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 [4]. Assuming constant density and viscosity, the Navier-Stokes equation can be rewritten as:

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

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

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

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

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

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

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

Introducing this expression to the integrated equation:

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

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

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

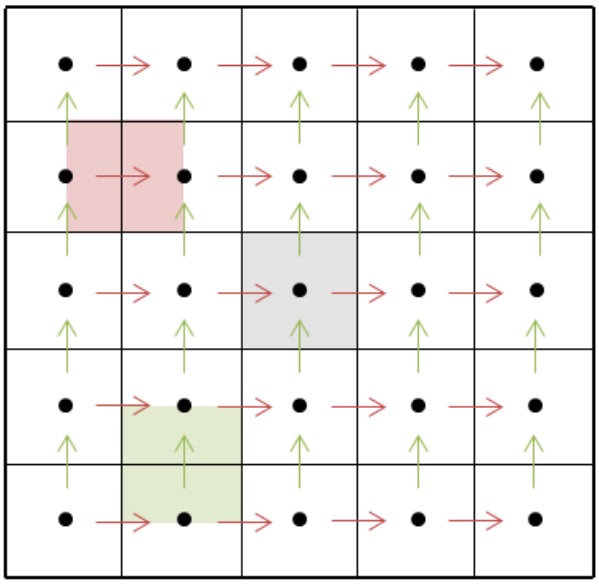


Figure 7.1: Staggered meshes (2D)

## 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, this method 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.

## 7.2 Discretization

To avoid convergence problems or incorrect solutions, 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. Knowing the space discretization of the domain, the discretized Poisson equation can be calculated.

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

$$\frac{p_E^{n+1}-p_P^{n+1}}{d_{EP}}A_e+\frac{p_N^{n+1}-p_P^{n+1}}{d_{NP}}A_n-\frac{p_P^{n+1}-p_W^{n+1}}{d_{WP}}A_w-\frac{p_P^{n+1}-p_S^{n+1}}{d_{SP}}A_s= \frac{1}{\Delta t}\left[\left(\rho u^P\right)_e A_e+\left(\rho v^P\right)_n A_n-\left(\rho u^P\right)_w A_w-\left(\rho v^P\right)_s A_s\right] \tag{7.8}$$

Rewriting the equation using discretization coefficients:

$$a_P p_P^{n+1}=a_E p_E^{n+1}+a_W p_W^{n+1}+a_N p_N^{n+1}+a_S p_S^{n+1}+b_P \tag{7.9}$$

where

$$a_P=a_E+a_W+a_N+a_S \tag{7.10}$$

$$a_E=\frac{A_e}{d_{EP}} \tag{7.11}$$

$$a_W=\frac{A_w}{d_{WP}} \tag{7.12}$$

$$a_N=\frac{A_n}{d_{NP}} \tag{7.13}$$

$$a_S=\frac{A_s}{d_{SP}} \tag{7.14}$$

$$b_P=-\frac{1}{\Delta t}\left[\left(\rho u^P\right)_e A_e+\left(\rho v^P\right)_n A_n-\left(\rho u^P\right)_w A_w-\left(\rho v^P\right)_s A_s\right] \tag{7.15}$$

# 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.

## 8.1 Boundary conditions

It is necessary to impose the conditions defined by figure 8.1. These boundary conditions modify the discretization coefficients in the boundary nodes. 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:

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

$$P_P = p_E \tag{8.2}$$

The prescribed velocity is defined using a similar approach. It is assumed that $u_P^{n+1} = u^P$. To obtain this solution, the pressure gradient has to be equal to zero, so the same expression as in the boundary layer conditions is obtained.

| 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 8.1: Discretization coefficients in the boundary

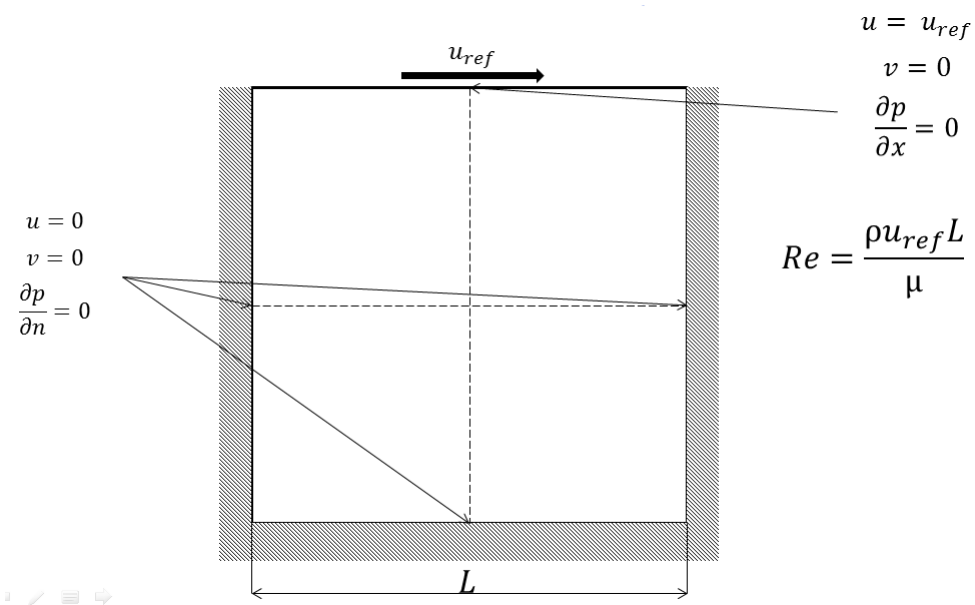



Figure 8.1: General scheme of the driven cavity problem

# 9 | Bibliography

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[3] Theodore L. Bergman, Adrienne S. Lavine, Frank P. Incropera, and David P. DeWitt. *Fundamentals of Heat and Mass Transfer*. John Wiley & Sons, 7 edition, 2011.

[4] CTTC. Introduction to the Fractional Step Method. pages 1–10.