ESEIAAT - UPC

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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1.1 Introduction

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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:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \tag{2.1.1}$$

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v}\vec{v}) = -\nabla p + \nabla \cdot \vec{\tau} + \rho \vec{g} + \vec{f}^e \tag{2.1.2}$$

$$\frac{\partial}{\partial t}(\rho u) + \nabla \cdot (\rho \vec{v} u) = -\nabla \cdot \vec{q} - p\nabla \cdot \vec{v} + \vec{\tau} : \nabla \vec{v} + \Phi^e \tag{2.1.3}$$

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

$$\rho c_p \left(\frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T \right) = \nabla \cdot (\lambda \nabla T) \tag{2.1.4}$$

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

$$\frac{\partial}{\partial t}(\rho \phi) + \nabla \cdot (\rho \vec{v} \phi) = \nabla \cdot (\Gamma \nabla \phi) + S_{phi} \tag{2.1.5}$$

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 2.1.1.

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

Table 2.1.1: 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.

2.2.1 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 2.2.1, the approximation of the values in the left point (west) and in the right point (east) is easily calculated with Taylor series:

$$\phi_W = \phi_P - \Delta x \left(\frac{d\phi}{dx}\right)_P + \frac{1}{2}(\Delta x)^2 \left(\frac{d^2\phi}{dx^2}\right) - \ldots \tag{2.2.1}$$

$$\phi_E = \phi_P + \Delta x \left(\frac{d\phi}{dx}\right)_P + \frac{1}{2}(\Delta x)^2 \left(\frac{d^2\phi}{dx^2}\right) + \ldots \tag{2.2.2}$$

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

$$\left(\frac{d\phi}{dx}\right)_P \approx \frac{\phi_E - \phi_W}{2\Delta x} \tag{2.2.3}$$

$$\left(\frac{d^2\phi}{dx^2}\right)_P \approx \frac{\phi_W + \phi_E - 2\phi_P}{(\Delta x)^2} \tag{2.2.4}$$

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.

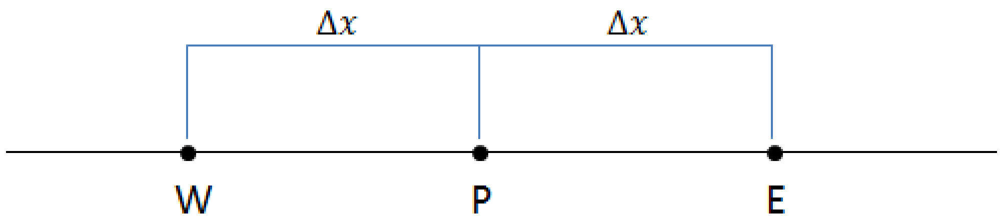

Figure 2.2.1: Three successive grid points

2.2.2 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 2.2.2, 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.

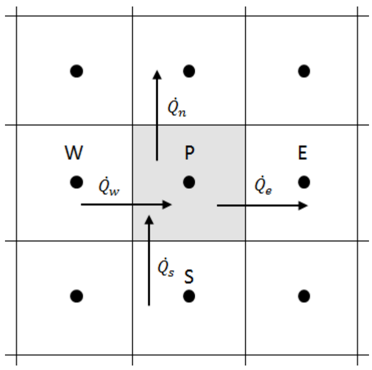

Figure 2.2.2: Control volume (2D)

2.2.3 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.

2.3 Evaluation of the convective term

There are different schemes to evaluate the convective term of the convection-diffusion equation. This term is evaluated in the faces, not in the nodes, so it is necessary to know the value in the faces of the control volume. Some of the most common schemes are listed below [2, 3], all of them studied in a one-dimensional case to simplify their explanation.

2.3.1 The central differencing scheme (CDS)

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

$$\phi_e - \phi_P = \frac{d_{Pe}}{d_{PE}} (\phi_E - \phi_P) \tag{2.3.1}$$

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

2.3.2 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.

$$\begin{aligned} \phi_e &= \phi_P, \quad \text{if } \dot{m}_e > 0 \\ \phi_e &= \phi_E, \quad \text{if } \dot{m}_e < 0 \end{aligned} \tag{2.3.2}$$

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.

2.3.3 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:

$$\frac{\phi - \phi_0}{\phi_L - \phi_0} = \frac{exp\,(Px/L) - 1}{exp\,(P) - 1} \tag{2.3.3}$$

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:

$$P \equiv \frac{\rho u L}{\Gamma} \tag{2.3.4}$$

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

$$\phi_e - \phi_P = \frac{exp\left(P_e d_{Pe}/d_{PE}\right) - 1}{exp\left(P_e\right) - 1}\left(\phi_E - \phi_P\right) \tag{2.3.5}$$

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.

2.3.4 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.

3 Conduction

The conduction heat transfer is described by Equation 3.0.1:

$$\rho c_P \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + \dot{q}_v \tag{3.0.1}$$

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

3.1 Four materials

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 3.1.1.

	x [m]	y [m]
p_1	0.50	0.40
p_2	0.50	0.70
p_3	1.10	0.80

Table 3.1.1: 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 3.1.2: Physical properties of the materials

The initial temperature field is $T = 8.00žC$.

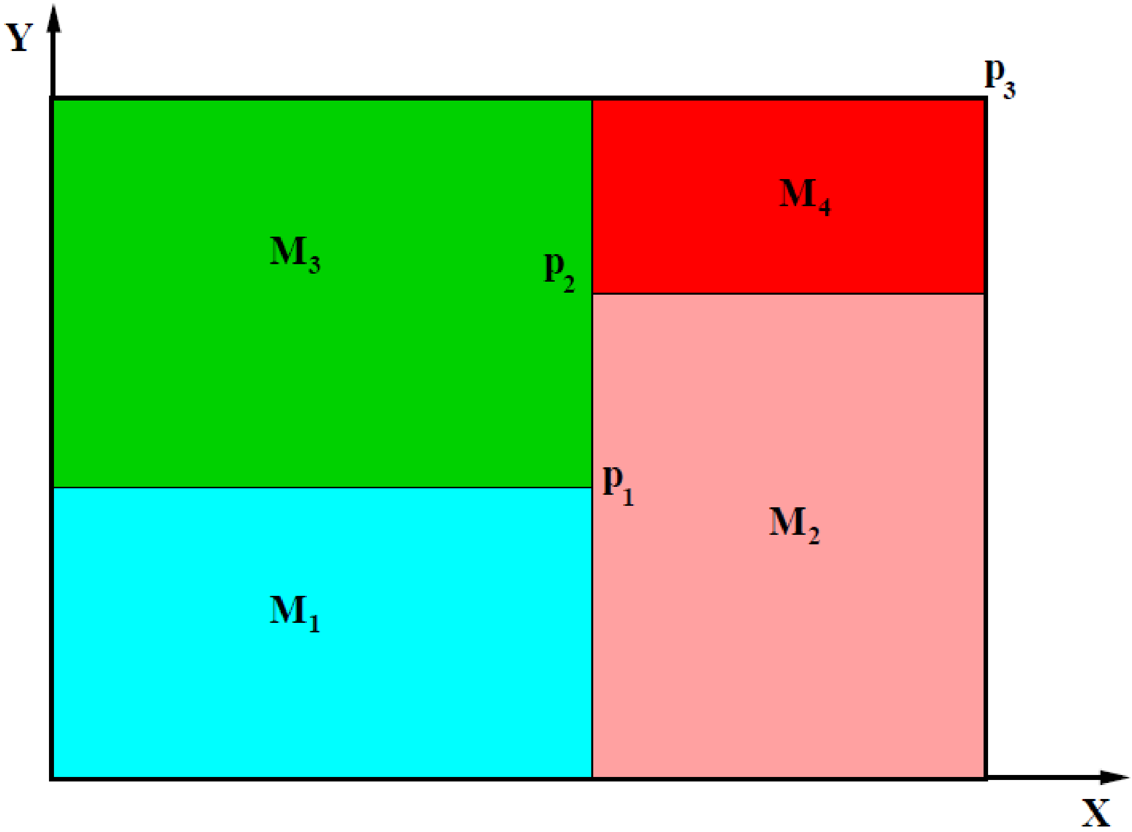

Figure 3.1.1: General scheme of the four materials problem

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

Table 3.1.3: Boundary conditions

3.2 Discretization

The domain is discretized using the node centred distribution, to avoid having conflictive control volumes between the different materials. Since it is a transitory problem, it is necessary to discretize in space and time. The method used to discretize the equation is the finite volume method.

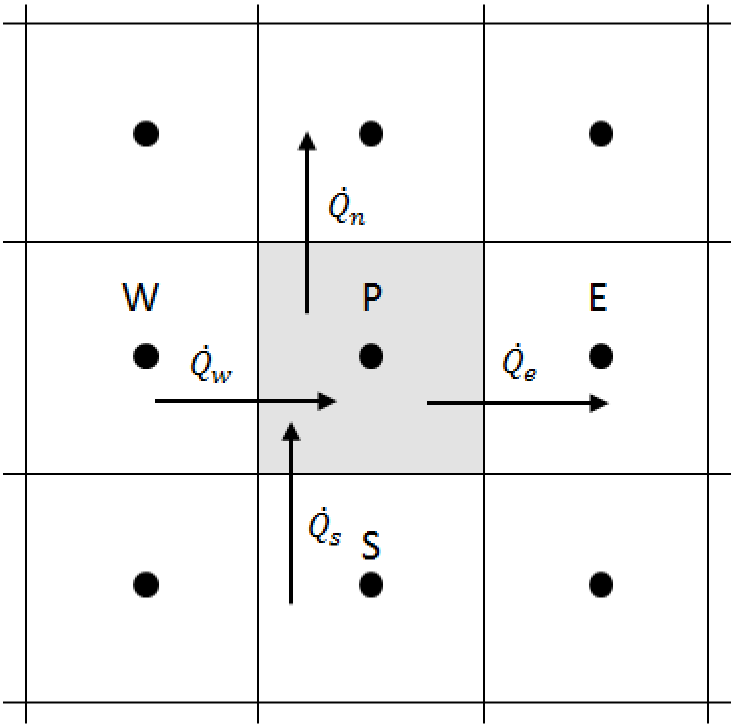

Figure 3.2.1: Heat fluxes through the faces of a control volume

3.2.1 Spatial discretization

The heat fluxes through the walls represented in figure 3.2.1 are integrated:

$$\dot{Q}_e = -\int^{S_e} \lambda \frac{\partial T}{\partial x} dS \approx -\left(\lambda \frac{\partial T}{\partial x}\right)_e S_e \approx -\lambda_e \frac{T_E - T_P}{d_{PE}} S_e \tag{3.2.1}$$

$$\dot{Q}_w = -\int^{S_w} \lambda \frac{\partial T}{\partial x} dS \approx -\left(\lambda \frac{\partial T}{\partial x}\right)_w S_w \approx -\lambda_w \frac{T_P - T_W}{d_{PW}} S_w \tag{3.2.2}$$

$$\dot{Q}_n = -\int^{S_n} \lambda \frac{\partial T}{\partial x} dS \approx -\left(\lambda \frac{\partial T}{\partial x}\right)_n S_n \approx -\lambda_n \frac{T_N - T_P}{d_{PN}} S_n \tag{3.2.3}$$

$$\dot{Q}_s = -\int^{S_s} \lambda \frac{\partial T}{\partial x} dS \approx -\left(\lambda \frac{\partial T}{\partial x}\right)_s S_s \approx -\lambda_s \frac{T_P - T_S}{d_{PS}} S_s \tag{3.2.4}$$

where T is the temperature at the given node, d the distance between two nodes, and λ the conductivity at the given face. However, since there are different materials there are faces in which the conductivity can have two values: one on the left side of the face and the other one on the right side of the face. This problem is solved with the harmonic mean. It can be calculated with the heat fluxes through the wall:

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

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

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

$$\lambda_e = \frac{d_{PE}}{\frac{d_{Pe}}{\lambda_P} + \frac{d_{Ee}}{\lambda_E}} \tag{3.2.5}$$

The inner heat of the material can be discretized as:

$$Q_{VP} = \int_{V_P} \dot{q}_v dV \approx \dot{q}_{vP} V_P \tag{3.2.6}$$

3.2.2 Time discretization

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

$$\int_{V_P} \rho \frac{\partial u}{\partial t} dV = \sum \dot{Q}_P \tag{3.2.7}$$

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:

$$\int_{t^n}^{t^{n+1}} \rho_P \frac{\partial \bar{u}_P}{\partial t} V_P dt = \int_{t^n}^{t^{n+1}} \sum \dot{Q}_P dt \tag{3.2.8}$$

Rearranging the first term of the equation:

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

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

The discretized equation is finally obtained:

$$\rho_P V_P \bar{c}_P \frac{T_P^{n+1} - T_P^n}{\Delta t} = \beta \left[-\lambda_w \frac{T_P - T_W}{d_{PW}} S_w + \lambda_e \frac{T_E - T_P}{d_{PE}} S_e - \lambda_s \frac{T_P - T_S}{d_{PS}} S_s + \lambda_n \frac{T_N - T_P}{d_{PN}} S_n + \dot{q}_{vP} V_P \right]^{n+1} + \tag{3.2.9}$$

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

$$a_P T_P = a_E T_E + a_W T_W + a_N T_N + a_S T_S + b_P \tag{3.2.10}$$

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

$$a_E = \beta \frac{\lambda_e S_e}{d_{PE}} \tag{3.2.11}$$

$$a_W = \beta \frac{\lambda_w S_w}{d_{PW}} \tag{3.2.12}$$

$$a_N = \beta \frac{\lambda_n S_n}{d_{PN}} \tag{3.2.13}$$

$$a_S = \beta \frac{\lambda_s S_s}{d_{PS}} \tag{3.2.14}$$

$$a_P = a_E + a_W + a_N + a_S + \rho_P V_P \bar{c}_P / \Delta t \tag{3.2.15}$$

$$b_P = \frac{\rho_P V_P \bar{c}_P T_P^n}{\Delta t} + \beta \dot{q}_{vP}^{n+1} V_P + (1-\beta)\left[-\lambda_w \frac{T_P - T_W}{d_{PW}} S_w + \lambda_e \frac{T_E - T_P}{d_{PE}} S_e - \lambda_s \frac{T_P - T_S}{d_{PS}} S_s + \lambda_n \frac{T_N - T_P}{d_{PN}} S_n + \right. \tag{3.2.16}$$

3.2.3 Boundary conditions

The outer walls of the rod have special conditions, so each of them has to be studied in order to determine the coefficients of the boundary nodes. In the left wall, there is convection, so some coefficients have to be recalculated:

$$a_W = 0 \tag{3.2.17}$$

$$a_P = a_E + a_W + a_N + a_S + \frac{\rho_P V_P \bar{c}_P}{\Delta t} + \frac{\beta}{\frac{1}{\alpha} + \frac{d_{Pw}}{\lambda_P}} \tag{3.2.18}$$

$$b_P = \frac{\rho_P V_P \bar{c}_P T_P^n}{\Delta t} + \beta \left(\dot{q}_{vP}^{n+1} V_P + \frac{T_g}{\frac{1}{\alpha} + \frac{d_{Pw}}{\lambda_P}} \right) + (1-\beta)\left[\frac{T_g - T_P}{\frac{1}{\alpha} + \frac{d_{Pw}}{\lambda_P}} + \lambda_e \frac{T_E - T_P}{d_{PE}} S_e - \lambda_s \frac{T_P - T_S}{d_{PS}} S_s + \lambda_n \frac{T_N - T}{d_{PN}} \right. \tag{3.2.19}$$

In the top wall there is a constant heat flux. The new coefficients are:

$$a_N = 0 \tag{3.2.20}$$

$$b_P = \frac{\rho_P V_P \bar{c}_P T_P^n}{\Delta t} + \beta \dot{q}_{vP}^{n+1} V_P + Q_{flow} \frac{S_n}{S_{top}} + (1-\beta)\left[-\lambda_w \frac{T_P - T_W}{d_{PW}} S_w + \lambda_e \frac{T_E - T_P}{d_{PE}} S_e - \lambda_s \frac{T_P - T_S}{d_{PS}} S_s + \dot{q}_{vP} V \right. \tag{3.2.21}$$

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:

$$a_E = 0 \tag{3.2.22}$$

$$a_P = a_E + a_W + a_N + a_S + \frac{\rho_P V_P \bar{c}_P}{\Delta t} + \beta \frac{\lambda_P S_e}{d_{Pe}} \tag{3.2.23}$$

$$b_P = \frac{\rho_P V_P \bar{c}_P T_P^n}{\Delta t} + \beta \left(\dot{q}_{vP}^{n+1} V_P + \frac{\lambda_P S_e}{d_{Pe}} T_r^{n+1} \right) + (1-\beta)\left[-\lambda_w \frac{T_P - T_W}{d_{PW}} S_w + \lambda_P \frac{T_r - T_P}{d_{Pe}} S_e - \lambda_s \frac{T_P - T_S}{d_{PS}} S_s + \right. \tag{3.2.24}$$

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

$$a_S = 0 \tag{3.2.25}$$

$$a_P = a_E + a_W + a_N + a_S + \frac{\rho_P V_P \bar{c}_P}{\Delta t} + \beta \frac{\lambda_P S_s}{d_{Ps}} \tag{3.2.26}$$

$$b_P = \frac{\rho_P V_P \bar{c}_P T_P^n}{\Delta t} + \beta \left(\dot{q}_{vP}^{n+1} V_P + \frac{\lambda_P S_s}{d_{Ps}} T_b \right) + (1-\beta) \left[-\lambda_w \frac{T_P - T_W}{d_{PW}} S_w + \lambda_e \frac{T_E - T_P}{d_{PE}} S_e - \lambda_P \frac{T_P - T_b}{d_{Ps}} S_s + \lambda_n \right. \tag{3.2.27}$$

4 Convection

The mathematical formulation needed to solve this problem is the convection diffusion-equation 4.0.1:

$$\frac{\partial}{\partial t}(\rho\phi) + \nabla\cdot(\rho\vec{v}\phi) = \nabla\cdot(\Gamma\nabla\phi) + S_{phi} \tag{4.0.1}$$

4.1 Smith-Hutton problem

The Smith-Hutton problem is a two-dimensional steady convection-diffusion problem, represented in figure 4.1.1: The velocity field is given by equations 4.1.1 and 4.1.2:

$$u(x,y) = 2y\left(1-x^2\right) \tag{4.1.1}$$

$$v(x,y) = -2x\left(1-y^2\right) \tag{4.1.2}$$

And the prescribed boundary conditions for the variable ϕ are described in equation 4.1.3:

$$\begin{aligned} \phi &= 1+\tanh\left(\alpha\left(2x+1\right)\right), && y=0; x\in(-1,0)\,(inlet) \\ \frac{\partial\phi}{\partial y} &= 0, && x=0; y\in(-1,0)\,(outlet) \\ \phi &= 1-\tanh\left(\alpha\right), && (elsewhere) \end{aligned} \tag{4.1.3}$$

where $\alpha = 10$.

4.2 Discretization

It is necessary to discretize equation 4.0.1 in space and time. The control volume used to discretize the problem is specified in figure 4.2.1. 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 4.2.1:

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\vec{v}) = 0 \tag{4.2.1}$$

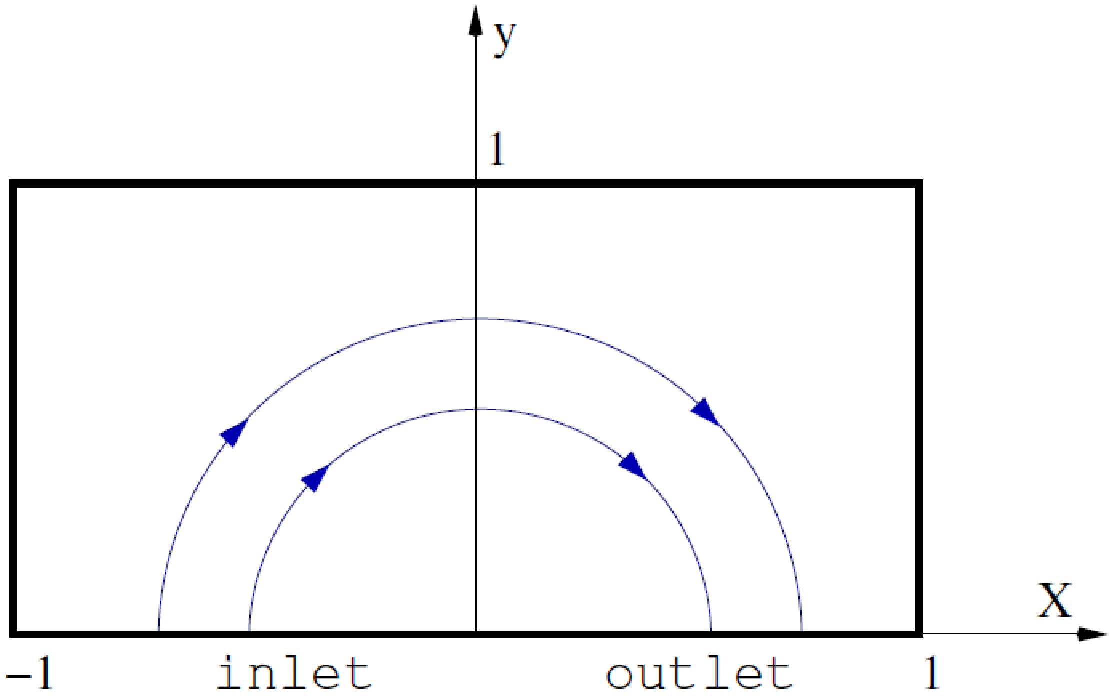

Figure 4.1.1: General scheme of the Smith-Hutton problem

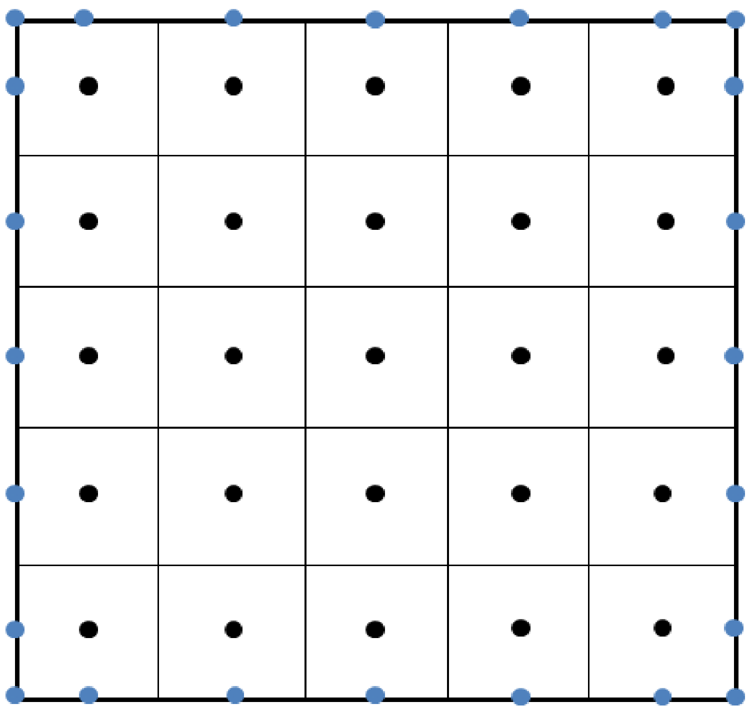

Figure 4.2.1: Mesh of the Smith-Hutton problem

The first step is to integrate Equation 4.2.1 over time and space. Taking only the first term of the equation:

$$\int_{t^n}^{t^{n+1}} \int_{V_P} \frac{\partial \rho}{\partial t} dV dt = \int_{t^n}^{t^{n+1}} V_P \frac{\partial \bar{\rho}_P}{\partial t} dt = V_P \left(\bar{\rho}_P^{n+1} - \bar{\rho}_P^n \right) \approx V_P \left(\rho_P^{n+1} - \rho_P^n \right) = V_P \left(\rho_P - \rho_0 \right) \tag{4.2.2}$$

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.

$$\int_{t^n}^{t^{n+1}} \int_{V_P} \nabla \cdot (\rho \vec{v})\, dV dt = \int_{t^n}^{t^{n+1}} \int_{S_f} \rho \vec{v} \cot \vec{n} dS dt = \int_{t^n}^{t^{n+1}} \left(\dot{m}_e - dotm_w + dotm_n - dotm_s \right) dt \approx \left[\dot{m}_e - dotm_w \right. \tag{4.2.3}$$

The final discretized mass equation is 4.2.4:

$$\frac{V_P \left(\rho_P - \rho_0 \right)}{\Delta t} + \dot{m}_e - dotm_w + dotm_n - dotm_s = 0 \tag{4.2.4}$$

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 4.0.1 and applying the Divergence Theorem:

$$\int_{V_P} \nabla \cdot (\rho \vec{v} \phi) = \int_{S_f} \rho \phi \vec{v} \cdot \vec{n} dS = \dot{m}_e \phi_e - \dot{m}_w \phi_w + \dot{m}_n \phi_n - \dot{m}_s \phi_s \tag{4.2.5}$$

The same procedure is used for the diffusion term of equation 4.0.1:

$$\int_{V_P} \nabla \cdot (\Gamma \nabla \phi) = \int_{S_f} \Gamma \cdot \nabla \phi \cdot \vec{n} dS = -\Gamma_w \frac{\partial \phi}{\partial x}\Big|_w S_w + \Gamma_e \frac{\partial \phi}{\partial x}\Big|_e S_e - \Gamma_s \frac{\partial \phi}{\partial x}\Big|_s S_s + \Gamma_n \frac{\partial \phi}{\partial x}\Big|_n S_n \approx D_e \left(\phi_E - \phi_P \right) - D_w \left(\phi_P \right. \tag{4.2.6}$$

where

$$D_e = \frac{\Gamma_e S_e}{d_{PE}} \tag{4.2.7}$$

$$D_w = \frac{\Gamma_w S_w}{d_{PW}} \tag{4.2.8}$$

$$D_n = \frac{\Gamma_n S_n}{d_{PN}} \tag{4.2.9}$$

$$D_s = \frac{\Gamma_s S_s}{d_{PS}} \tag{4.2.10}$$

To simplify the source term, it is linearized:

$$\int_{V_P} S_\phi dV \approx S_{\phi,P} V_P = \left(S_c^\phi + S_p^\phi \phi_P \right) V_P \tag{4.2.11}$$

So that the resulting discretized equation is:

$$\frac{\rho_P \phi_P - \rho_P^0 \phi_P^0}{\Delta t} V_P + \dot{m}_e \phi_e - \dot{m}_w \phi_w + \dot{m}_n \phi_n - \dot{m}_s \phi_s = D_e \left(\phi_E - \phi_P \right) - D_w \left(\phi_P - \phi_W \right) + D_n \left(\phi_N - \phi_P \right) - D_s \left(\phi_P - \right. \tag{4.2.12}$$

Multiplying by ϕ the discretized mass equation 4.2.4 and subtracting the result in 4.2.12, the discretized convection-diffusion equation is obtained:

$$\rho_P^0 \frac{\phi_P - \phi_P^0}{\Delta t} V_P + \dot{m}_e \left(\phi_e - \phi_P\right) - \dot{m}_w \left(\phi_w - \phi_P\right) + \dot{m}_n \left(\phi_n - \phi_P\right) - \dot{m}_s \left(\phi_s - \phi_P\right) = D_e \left(\phi_E - \phi_P\right) - D_w \left(\phi_P - \phi_W \right. \tag{4.2.13}$$

To simplify the problem, a new variable is introduced to the problem: the total flux [3]. 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.

$$J_x \equiv \rho u \phi - \Gamma \frac{\partial \phi}{\partial x} \tag{4.2.14}$$

$$J_y \equiv \rho v \phi - \Gamma \frac{\partial \phi}{\partial y} \tag{4.2.15}$$

Introducing the expressions of the total flux 4.2.14 and 4.2.15 to 4.2.13, the discretized convection diffusion equation becomes:

$$\rho_P^0 \frac{\phi_P - \phi_P^0}{\Delta t} V_P + \left(J_e - F_e \phi_P\right) - \left(J_w - F_w \phi_P\right) + \left(J_n - F_n \phi_P\right) - \left(J_s - F_s \phi_P\right) = \left(S_p^\phi \phi_P\right) V_P \tag{4.2.16}$$

where the flow rates are:

$$F_e = \left(\rho u\right)_e S_e \tag{4.2.17}$$

$$F_w = \left(\rho u\right)_w S_w \tag{4.2.18}$$

$$F_n = \left(\rho v\right)_n S_n \tag{4.2.19}$$

$$F_s = \left(\rho v\right)_s S_s \tag{4.2.20}$$

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:

$$J^* \equiv \frac{J\delta}{\Gamma} = P\phi - \frac{d\phi}{d\left(x/\delta\right)} \tag{4.2.21}$$

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 $d\phi/d\left(x/\delta\right)$ are a combination of the ϕ_i and ϕ_{i+1}, so that J^* can be expressed as [3]:

$$J^* = B\phi_i - A\phi_{i+1} \tag{4.2.22}$$

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 [3]. Taking these properties into account and introducing the operator $[A, B]$ that denotes the greater of A and B, it can be deduced that:

$$A\left(P\right) = A\left(|P|\right) + \left[-P, 0\right] \tag{4.2.23}$$

$$B\left(P\right) = A\left(|P|\right) + \left[-P, 0\right] \tag{4.2.24}$$

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

Table 4.2.1: Function $A(|P|)$ for different schemes [?]

Introducing equations 4.2.23 and 4.2.24 into 4.2.16, the following formulation is obtained:

$$a_P\phi_P = a_E\phi_E + a_W\phi_W + a_N\phi_N + a_S\phi_S + b_P \tag{4.2.25}$$

where

$$a_E = D_eA\left(|P_e|\right) + [-F_e, 0] \tag{4.2.26}$$

$$a_W = D_wA\left(|P_w|\right) + [F_w, 0] \tag{4.2.27}$$

$$a_N = D_nA\left(|P_n|\right) + [-F_n, 0] \tag{4.2.28}$$

$$a_S = D_sA\left(|P_s|\right) + [-F_s, 0] \tag{4.2.29}$$

$$a_P = a_E + a_W + a_N + a_S + \frac{\rho_P^0 V_P}{\Delta t} - S_P V_P \tag{4.2.30}$$

$$b_P = S_c V_P + \frac{\rho_P^0 V_P}{\Delta t}\phi_P^0 \tag{4.2.31}$$

And the Péclet numbers are:

$$P_e = \frac{F_e}{D_e} \tag{4.2.32}$$

$$P_w = \frac{F_w}{D_w} \tag{4.2.33}$$

$$P_n = \frac{F_n}{D_n} \tag{4.2.34}$$

$$P_s = \frac{F_s}{D_s} \tag{4.2.35}$$

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 4.2.1.

4.3 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 4.3.1. The aim of the problem is to obtain the distribution of velocities inside the cavity.

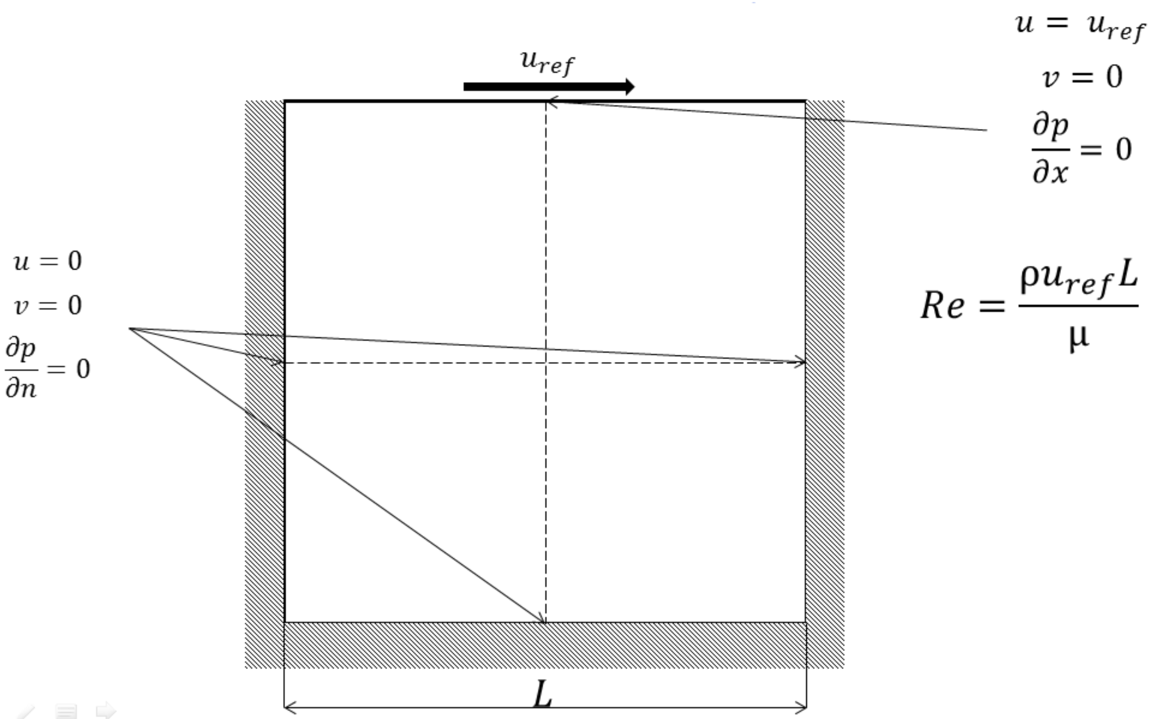

Figure 4.3.1: General scheme of the driven cavity problem

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

$$\begin{gathered}\nabla \cdot = 0 \\ \rho \frac{\partial \vec{v}}{\partial t} + \rho \left(\vec{v} \cdot \nabla\right) \vec{v} = -\nabla p + \mu \nabla^2 \vec{v}\end{gathered} \tag{4.3.1}$$

4.4 Fractional step method

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

$$\rho \frac{\partial \vec{v}}{\partial t} = R\left(\vec{v}\right) - \nabla p \tag{4.4.1}$$

where $R\left(\vec{v}\right) = -\rho\left(\vec{v} \cdot \nabla\right)\vec{v} + \mu \nabla^2 \vec{v}$. Integrating the equation 4.4.1 over time:

$$\rho \frac{\vec{v}^{n+1} - \vec{v}^{n}}{\Delta t} = R^{n+\frac{1}{2}}\left(\vec{v}\right) - \nabla p^{n+1} \tag{4.4.2}$$

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:

$$R^{n+\frac{1}{2}}\left(\vec{v}\right) \approx \frac{3}{2} R\left(\vec{v^{n}}\right) - \frac{1}{2} R\left(\vec{v}^{n-1}\right) \tag{4.4.3}$$

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

$$\vec{v}^P = \vec{v}^{n+1} + \frac{\Delta t}{\rho} \nabla p^{n+1} \tag{4.4.4}$$

Introducing this expression to the integrated equation:

$$\rho \frac{\vec{v}^P - \vec{v}^n}{\Delta t} = R^{n+\frac{1}{2}} \left(\vec{v} \right) \tag{4.4.5}$$

And finally, applying the divergence to the expression of the intermediate velocity $\vec{v}^P$ 4.4.4, the Poisson equation is obtained:

$$\nabla \cdot \vec{v} = \frac{\Delta t}{\rho} \nabla^2 p \tag{4.4.6}$$

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

1. Evaluate $R^{n+\frac{1}{2}} \left(\vec{v} \right)$.
2. Calculate the intermediate velocity with equation 4.4.5.
3. Calculate the pressure p^{n+1} from the Poisson equation 4.4.6 using a linear solver.
4. Calculate the velocity at the next time step with equation 4.4.4.

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.

4.5 Discretization

To avoid convergence problems or incorrect solutions, the staggered meshes are used. As shown in figure 4.5.1, 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:

$$\frac{p_E^{n+1} - p_P^{n+1}}{d_{EP}} A_e + \frac{p_N^{n+1} - p_P^{n+1}}{d_{NP}} A_n - \frac{p_P^{n+1} - p_W^{n+1}}{d_{WP}} A_w - \frac{p_P^{n+1} - p_S^{n+1}}{d_{SP}} A_s = \frac{1}{\Delta t} \left[\left(\rho u^P \right)_e A_e + \left(\rho v^P \right)_n A_n - \left(\rho u^P \right. \right. \tag{4.5.1}$$

Rewriting the equation using discretization coefficients:

$$a_P p_P^{n+1} = a_E p_E^{n+1} + a_W p_W^{n+1} + a_N p_N^{n+1} + a_S p_S^{n+1} + b_P \tag{4.5.2}$$

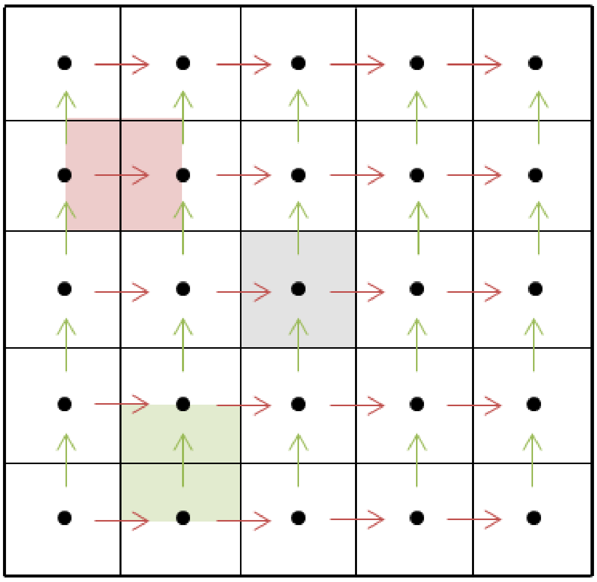

Figure 4.5.1: Staggered meshes (2D)

where

$$a_P = a_E + a_W + a_N + a_S \tag{4.5.3}$$

$$a_E = \frac{A_e}{d_{EP}} \tag{4.5.4}$$

$$a_W = \frac{A_w}{d_{WP}} \tag{4.5.5}$$

$$a_N = \frac{A_n}{d_{NP}} \tag{4.5.6}$$

$$a_S = \frac{A_s}{d_{SP}} \tag{4.5.7}$$

$$b_P = -\frac{1}{\Delta t}\left[\left(\rho u^P\right)_e A_e + \left(\rho v^P\right)_n A_n - \left(\rho u^P\right)_w A_w - \left(\rho v^P\right)_s A_s\right] \tag{4.5.8}$$

4.6 Boundary conditions

It is necessary to impose the conditions defined by figure 4.3.1. 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:

$$\frac{\partial p}{\partial x} \approx \frac{p_E - p_P}{\Delta x} = 0 \tag{4.6.1}$$

$$P_P = p_E \tag{4.6.2}$$

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 4.6.1: Discretization coefficients in the boundary

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.

5 Turbulence

5.1 Burgers equation

6 Radiation

7 | Bibliography

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

[2] Joel H. Ferziger and Milovan Peric. *Computational Methods for Fluid Dynamics*. Springer, Berlin, 3 edition, 2002.

[3] Suhas V. Patankar. *Numerical Heat Transfer and Fluid Flow*. McGraw-Hill, New York, 1980.