Smith-Hutton and numerical analysis of Convection-Diffusion case studies

Edgar Gago Carrillo

Polytechnic University of Catalonia, Barcelona, Spain
edgar.gago@upc.edu | edgargc.upc@gmail.com

November 1, 2020

Abstract — This report aims to provide an introduction to the solution of convection-diffusion problems using three case studies: parallel diagonal flow, and the Smith-Hutton case study. A MATLAB code has been developed in order to analyse the different case studies and prove the code's performance and quality.

1 Introduction

Many problems that involves the resolution of differential equations can be solved *analytically* specially those ones that involve simple geometries with simple boundary conditions. But when the problem involve complicated geometries with complex *boundary conditions* and variable properties its needed another method for solving the equations involved in the physical phenomenon.

For this cases we can still obtain sufficiently accurate approximate solutions using *numerical methods*, those are based on replacing the differential equation by a set of n algebraic equations for the unknown medium property at n selected points of the medium, and the simultaneous solution of these equation results in the medium property values at those *discrete points*. We are going to call this arbitrary medium property or dependent variable ϕ to refer to it in the following sections. [2]

The numerical solution of heat transfer, fluid flow, and other related processes can begin when the laws governing these processes have been expressed in mathematical form, generally in terms of differential equations. In this section we are going to develop the mathematical formulation and complete derivation of the convection-diffusion equation as an initial step for developing the code for modelling these phenomenon [3]. The purpose in this section is to develop the familiarity with the form and meaning of these equations, geometric formulation of the control volume and the main ingredients for developing the *numerical simulation* tools for the case of study.

Accurate modelling of the interaction between convective and diffusive processes is a challenging task in numerical approximation of partial differential equations. Many different ideas and approaches have been proposed in different contexts in order to resolve the difficulties such as exponential fitting, compact differences, upwind, etc. being some examples from the fields of finite difference and finite element methods.

It is important to know that mathematical models that involve a combination of convective and diffusive processes are among the most widespread in all of science, engineering and other fields where mathematical models are involved. The convection term has an inseparable connection with the diffusion term so they need to be handled as one unit but its formulation is not as simple as the diffusion phenomena. This chapter gives us a better understanding of the Navier-Stokes equations before treating the final equation that merges the convection and diffusion phenomena. [3]

2 Navier-Stokes Equations

Before starting the formulation of the Convection-Diffusion equation its important to have clear the meaning of each one of the ns equations. The ns equations consists of the continuity equation, which represents the mass conservation principle (Eq.1); the momentum conservation equations, one for each problem dimension (Eq.2); and the energy conservation equation (Eq.3). [4]

$$\frac{d\rho}{dt} + \nabla \cdot (\rho \overrightarrow{v}) = 0 \tag{1}$$

$$\frac{d}{dt}(\rho \overrightarrow{v}) + \nabla \cdot (\rho \overrightarrow{v} \overrightarrow{v}) = -\nabla p + \nabla \cdot (\overrightarrow{\tau}) + \rho \overrightarrow{g} \tag{2}$$

$$\frac{d}{dt}(\rho(u + e_c)) + \nabla \cdot ((u + e_c)\rho \overrightarrow{v}) = -\nabla \cdot (\rho \overrightarrow{v}) + \nabla(\overrightarrow{v} \cdot \overrightarrow{\tau}) - \nabla \cdot \overrightarrow{q} + \rho \overrightarrow{g} \cdot \overrightarrow{v} + G \tag{3}$$

Some previous assumptions have been done in the ns equations, this hypothesis are:

- Continuity of matter
- Continuum medium assumption
- Relativity effects negligible
- Inertial reference system
- Magnetic and electromagnetic forces negligible

Table **??** gives an accurate physical description in order to have a better understanding of the Navier-Stokes equations before starting to work with them.

3 Equation Formulation

The Convection-Diffusion equation is a combination of the conservation equations of mass, linear momentum and energy also called Navier-Stokes equations. The convection is created by fluid flow, our task is to obtain a solution for the general variable ϕ in the presence of a given flow field for a given diffusion coefficient Γ . Having somehow acquired the flow field the temperature, concentration, enthalpy, or any such quantity that is represented by the general variable ϕ could be easily calculated.

3.1 Simplified ns Equations

The ns explained in the previous section can be simplified for the conditions and assumptions related to our Convection-Diffusion equation formulation. [?] Then it can be found that the simplified ns equation that governs the flow of a Newtonian fluid in Cartesian coordinates assuming:

- 2d model
- Laminar flow
- Incompressible flow
- Newtonian fluid
- Boussinesq hypothesis[1]
- Negligible viscous dissipation
- Negligible compression or expansion work

[1]Constant physical properties everywhere except in the body forces term

- Non-participating medium in radiation
- Mono-component and mono-phase fluid

The use of constant properties of thermal conductivity, density... implies that it will not be possible to solve problems with a huge range in temperatures because all of these properties depend on it.

Simplifying equations from Eq.1 to 3:

$$\frac{du}{dx} + \frac{dv}{dy} = 0 \tag{4}$$

$$\rho\frac{du}{dx} + \rho u\frac{du}{dx} + \rho v\frac{du}{dy} = -\frac{dp}{dx} + \mu\Big(\frac{d^2u}{dx^2} + \frac{d^2u}{dy^2}\Big) \tag{5}$$

$$\rho\frac{du}{dx} + \rho u\frac{dv}{dx} + \rho v\frac{dv}{dy} = -\frac{dp}{dy} + \mu\Big(\frac{d^2v}{dx^2} + \frac{d^2v}{dy^2}\Big) + \rho g\beta(T - T_\infty) \tag{6}$$

$$\rho\frac{dT}{dt} + \rho u\frac{dT}{dx} + \rho v\frac{dT}{dy} = \frac{k}{c_p}\Big(\frac{d^2T}{dx^2} + \frac{d^2T}{dy^2}\Big) + \frac{G}{c_p} \tag{7}$$

Noting that in this equation there are four unknown values: pressure, temperature and the two components of velocity u and v. Furthermore, a boundary condition and an initial condition are required to solve the problem.

Analysing the system of equations closely it can be observed a strong coupling between them:

- Pressure - Velocity: for the previous established conditions, there is no specific pressure equation, but the pressure distribution allows the velocity field to satisfy the mass conservation equation.
- Temperature - Velocity: there is only a coupling characterisation for natural convection, mixed connection or when the physical properties depend on the temperature. In forced convection and constant physical properties, the velocity field does not depend on temperature field.

3.2 Convection-Diffusion Equation

Acknowledging the coupling from the partial differential equations and applying the corresponding assumptions all equations from Eq.(4 - 7) can be summarised into the convection-diffusion equation:

$$\frac{d(\rho\phi)}{dt} + \nabla(\rho\overrightarrow{v}\phi) = \nabla(\Gamma\nabla\phi) + G \tag{8}$$

in Cartesian coordinates, incompressible flow and constant physical properties the equation can also be written as

$$\rho\frac{d\phi}{dt} + \rho u\frac{d\phi}{dx} + \rho v\frac{d\phi}{dy} = \frac{k}{c_p}\Big(\frac{d^2\phi}{dx^2} + \frac{d^2\phi}{dy^2}\Big) + G \tag{9}$$

In the previous equation, the first term is the accumulation of ϕ which tells how ϕ change along time. The second and the third term are the net convective flow in the control volume, which gives information about the spatial transport of ϕ. The sum of these has to be equal to the net diffusive flow, which represents the transport of ϕ due to the concentration of gradients, plus the generation of ϕ per unit volume (G).

Looking at Eq.8 the *diffusion flux* due to the gradient of the general variable ϕ is $-\Gamma(d\phi/dx)$ where ϕ could represent chemical-species diffusion, heat flux, viscous stress, etc. According to Eq.8 a table with the parameters of ϕ, τ and G could be written in order to reproduce the governing equations (Eq. 4 - Eq. 7). Te values for the pressure, temperature and density field are obtained by introducing parameters of Table 1 into the ns equations once the field ϕ is solved.

Table 1: Parameters to obtain ns equations convection-diffusion equation

Equation	ϕ	τ	G
Continuity	1	0	0
Momentum in X direction	u	μ	$-dp/dx$
Momentum in Y direction	v	μ	$-dp/dy + \rho g \beta (T - T_\infty)$
Energy (constant c_p)	T	k/c_p	ϕ/c_p

4 Equation Discretization

In this section the implicit finite-volume discretization (fvm) of the convection-diffusion equation is shown. First of all Eq.9 has to be integrated into a rectangular cv.

$$\frac{(\rho\phi)_P^1 - (\rho\phi)_P^0}{\Delta t}\Delta x \Delta y + \Big[(\rho u \phi)_e^1 - (\rho u \phi)_w^1\Big]$$

$$\Delta y + \Big[(\rho v \phi)_n^1 - (\rho v \phi)_s^1\Big]\Delta x =$$

$$= \Big[\Big(\Gamma\frac{d\phi}{dx}\Big)_e^1 - \Big(\Gamma\frac{d\phi}{dx}\Big)_w^1\Big]\Delta y +$$

$$\Big[\Big(\Gamma\frac{d\phi}{dy}\Big)_n^1 - \Big(\Gamma\frac{d\phi}{dy}\Big)_s^1\Big]\Delta x + G_P^1 \Delta x \Delta y \quad (10)$$

Note that superindex "1" is used for the value of property ϕ at time $t = t + \Delta t$ and "0" at the previous time step value, for an easier formulation it can be stated that $\phi^1 = \phi$. Assuming $\Delta x \Delta y$ as the cv volume V_P and separately as their surfaces S_e , S_w, S_n and S_s

$$\frac{(\rho\phi)_P - (\rho\phi)_P^0}{\Delta t}V_P + \Big[(\rho u \phi)_e S_e - (\rho u \phi)_w S_w\Big]$$

$$+ \Big[(\rho v \phi)_n^1 S_n - (\rho v \phi)_s S_s\Big] =$$

$$= \Big[\Big(\Gamma\frac{d\phi}{dx}\Big)_e S_e - \Big(\Gamma\frac{d\phi}{dx}\Big)_w S_w\Big] + \Big[\Big(\Gamma\frac{d\phi}{dy}\Big)_n S_n -$$

$$\Big(\Gamma\frac{d\phi}{dy}\Big)_s S_s\Big] + G_P V_P \quad (11)$$

This formulation can be simplified using the total flux term, defined by:

$$J_x = \rho v \phi - \Gamma\frac{d\phi}{dx} \quad (12a)$$

$$J_y = \rho v \phi - \Gamma\frac{d\phi}{dy} \quad (12b)$$

Equation 8 can be expressed with the flux term J as:

$$\frac{d(\rho\phi)}{dt} + \frac{dJ_x}{dx} + \frac{dJ_y}{dy} = G \quad (13)$$

Integrating the previous equation into a rectangular cv and assuming an implicit scheme for the temporal integration, Eq. 13 yields to:

$$\frac{(\rho\phi)_P - (\rho\phi)_P^0}{\Delta t}V_P + J_e - J_w + J_n - J_s$$
$$= (G_c + G_P \phi_P)V_P \quad (14)$$

The quantities J_e , J_w , J_s and J_n are the integrated total fluxes over the control-volume faces; that is, J_e stands for $\int J_x dy$ over the interface e and so on. The source term has been linearized as it could be seen in the last term of Eq. 14.

Noting that the flow field has to satisfy the continuity equation (Eq. 4) in order to assume convergence:

$$\frac{d}{dx_j}(\rho u_j) = 0 \tag{15}$$

Integrating over a rectangular finite volume:

$$\frac{\rho_P - \rho_P^0}{\Delta t} V_P + F_e - F_w + F_n - F_s = 0 \tag{16}$$

where F_e, F_n, F_s and F_w are the mass flow rates through the faces of the cv.

$$F_e = (\rho u)_e S_e \tag{17a}$$

$$F_w = (\rho u)_w S_w \tag{17b}$$

$$F_n = (\rho v)_n S_n \tag{17c}$$

$$F_s = (\rho v)_s S_s \tag{17d}$$

Multiplying Eq.16 by ϕ_P and subtracting it from Eq.14:

$$(\phi_P - \phi_P^0)\frac{\rho_P^0}{\Delta t} \cdot V_P + (J_e - F_e\phi_P) - (J_w - F_w\phi_P) + \\ + (J_n - F_n\phi_P) - (J_s - F_s\phi_P) = (S_c + S_P\phi_P) \tag{18}$$

The assumption of uniformity over a control-volume face enables to employ 1d practices from Ref. [3] for the 2d situation.

5 Code

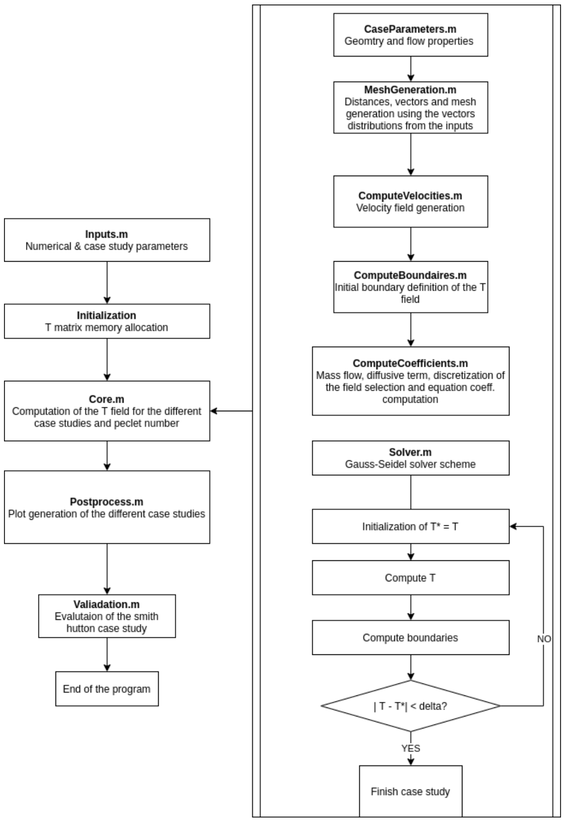


Figure 1: Problem's algorithm

(Fig. 1) shows problem's algorithm and the main functions and what do they do of the developed program. A higher resolution picture of the algorithm can be found here: algorithm source.

6 Evaluation schemes & the Peclet number

Evaluation schemes have an important impact on the computation of the weighting parameters. Two different schemes have been taken into account in order to present the code results:

- Upwind Differencing Scheme **UDS**: a first order scheme which is highly stable but due to being first order accurate may cause some errors.

$$f = 1 \tag{19}$$

- Exponential Differencing Scheme **(EDS)**: also a first order scheme but having its f parameter as function of the Péclet number.

$$f = \frac{|Pe|}{e^{|Pe-1|}} \tag{20}$$

The Péclet number is an adimensional number used in fluid mechanics which relates the advective and diffusive strength of the thermal flow. This relation can be written as:

$$Pe = \frac{Advective}{Diffusive} = \frac{\rho u L}{\mu} \tag{21}$$

In order to analyze the impact of the Péclet number onto the convection-diffusion behaviour, three different values are going to be taken into account as proposed in [1]. Thus, the simulation will be computed for the following Pe numbers:

- $Pe = 10, 10^3 and 10^6$

Even though the code is prepared to compute both schemes only the results for the UDS will be presented due to time constrains.

7 Parallel flow

This problem consists in the study of a one-dimensional flow with a one-dimensional variation of the variable solved in the same direction of the flow.

The parallel flow is treated in a squared symmetrical domain of size L with a velocity field of u = u0 and v = 0, which means horizontal velocity will be taken into account.
Considering the problem discussion made on the appendices, the convection-diffusion can be written as:

$$\rho\frac{d\phi}{dt}+\rho u\frac{d\phi}{dx}+\rho v\frac{d\phi}{dy} = \frac{k}{c_p}\left(\frac{d^2\phi}{dx^2}+\frac{d^2\phi}{dy^2}\right) \tag{22}$$

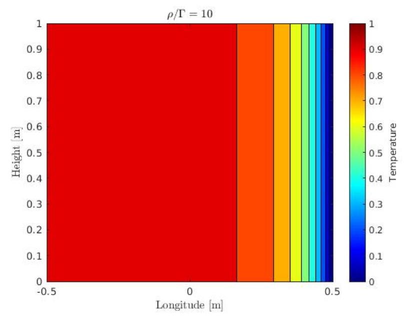
Note that, (Eq. 22), does not include the source term as the problem will be considered as steady.
The final solution of the discredited equation of (Eq. 22) can be written as:

$$a_P\phi_P = a_E\phi_E + a_S\phi_S + a_W\phi_W + a_N\phi_N + b \tag{23}$$

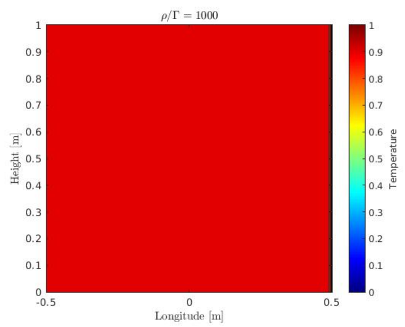
Where ϕ is a generic field variable and will represent the Temperature in this case study.

7.1 Results

The results showed the expected behaviour for a 1d dimensional problem. Interestingly for a EDS scheme the result converge faster than for the the UDS. The following pictures show the obtained results for different Péclet number and a mesh of 200 x 200 nodes without taking into account the boundaries.



(a) $Pe = 10$



(b) $Pe = 10^3, 10^6$

Figure 2: Obtained results for the parallel flow

Note that only two figures are presented. This because the results for the $Pe = 10^3$

and for the $Pe = 10^6$ where practically the same and no difference could be seen. This is because the advective forces, which are the ones that transport the fluid, star to be so big that from that point no matter the if it is 1000 or 10^6 times. An extra simulation was done with a $Pe = 100$, in that case it was possible to see the difference, but still the difference was not very big.

The obtained results make physical sense as the forces that moves the flow are higher it is expected that that propagation of the higher temperature, which in our case is the left side, domains as the flow velocity has a positive direction in the x axis.

8 Diagonal flow

For the diagonal flow the same discretization equation as in the parallel flow can be applied. The most important changes are the boundary and the velocity field, both can be find on the following listing:

- Boundary conditions:

$$T_{right} = T_{Bottom} = T_{Low} \tag{24}$$

$$T_{left} = T_{Top} = T_{High} \tag{25}$$

- Velocity field

$$\vec{v_x} = u_0 * sin(\alpha); \tag{26}$$

$$\vec{v_y} = u_0 * sin(\alpha); \tag{27}$$

Where $\alpha = 45$ as express on the class slides and the values for the upper and lower temperatures were taken as 1 and 0 respectively. The value of the temperatures do not change the final results, only alters the heat-map as it is automatically generated using a MATLAB function.

8.1 Results

The obtained results can be seen in the following pictures:

As it can be seen in all the (Fig. 10) the results are as expected. As a diagonal flow is applied inside the volume it can be clearly seen how the transition from hotter to colder is made diagonally. In this case study it can be better observed the change between the different Péclet numbers. As this number increases the diffusive forces are lower, therefore the transitions is made more abruptly.

Even tough the difference is slightly higher than in the previous case study, the difference between $Pe = 10^3$ and $Pe = 10^6$ is still really small.

9 Smith-Hutton

Finally the third case study will take into account a particular scenario which is the Smith-Hutton problem.The Smith-Hutton problem is treated in a rectangular domain of 2L × L and a known velocity field in its two components given by:

$$v_x = 2y(1 - x^2) \tag{28}$$

$$v_y = -2x(1 - y^2) \tag{29}$$

Velocity field which varies the incompressibility condition of

$$\nabla v = 0 \tag{30}$$

The boundary conditions for this problem are defined as follows:

$$\phi_{inlet} = 1 + tanh(\alpha(2x + 1)) \tag{31}$$

$$boundary_{outlet} = \frac{\partial \phi}{\partial y} = 0 \tag{32}$$

$$\phi_{left} = \phi_{top} = \phi_{right} = 1 - tanh(\alpha) \tag{33}$$

A representation of the Smith-Hutton problem is shown in the following picture:

9.1 Validation

In order to validate the code results, two different cases for different mesh sizes are going to be presented againts the following numerical results presented in one of the class documents:

Position x	$\rho/\Gamma = 10$	$\rho/\Gamma = 1000$	$\rho/\Gamma = 1000000$
0.0	1.989	2.0000	2.000
0.1	1.402	1.9990	2.000
0.2	1.146	1.9997	2.000
0.3	0.946	1.9850	1.999
0.4	0.775	1.8410	1.964
0.5	0.621	0.9510	1.000
0.6	0.480	0 1540	0.036
0.7	0.349	0.0010	0.001
0.8	0.227	0.0000	0.000
0.9	0.111	0.0000	0.000
1.0	0.000	0.0000	0.000

Figure 5: Given numerical results for different Péclet numbers

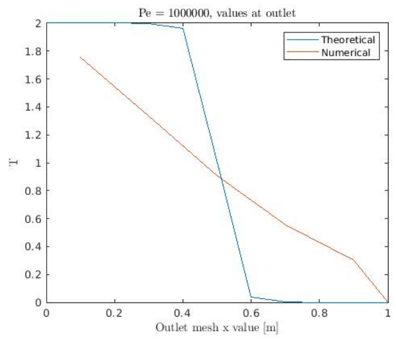


Figure 6: $Meshsize = 10$

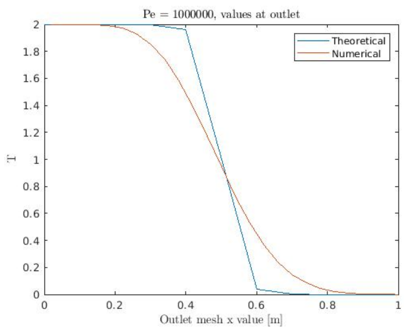


Figure 7: $Meshsize = 50$

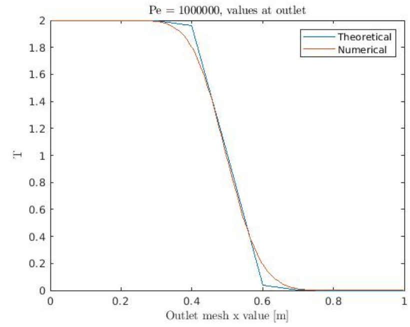


Figure 8: $Meshsize = 200$

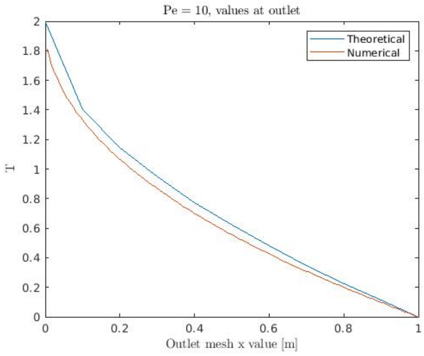
On the first validation made three mesh sized where taken into account:

- $M = 10$
- $M = 50$
- $M = 200$

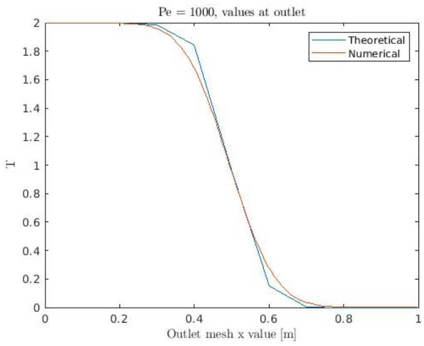
Using this three mesh size and a Péclet number of 10^6 was taken. This first iteration is made in order to see the mesh level that needs to be chosen so the results are as closed as possible and the validation can be chosen as correct.

On the graphics of the (Fig. 6-8) it can be seen how the higher the mesh resolution the better the solution. Taken these results into account a mesh size of 200 was selected in order to validate the results for the different Péclet numbers.

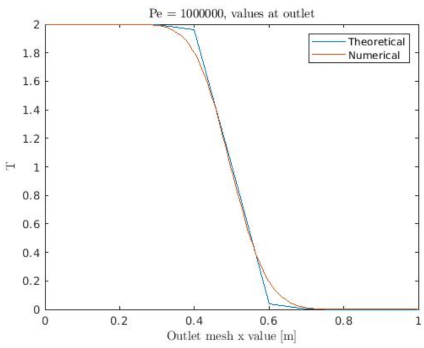
Note that for a higher number of divisions the results could have been even closer, but in terms of performance the error chosen it is acceptable as a higher mesh size would suppose a higher computational time.



(a) $Pe = 10$



(b) $Pe = 10^3$



(c) $Pe = 10^6$

Figure 9: Code validation using the Smith-Hutton case study

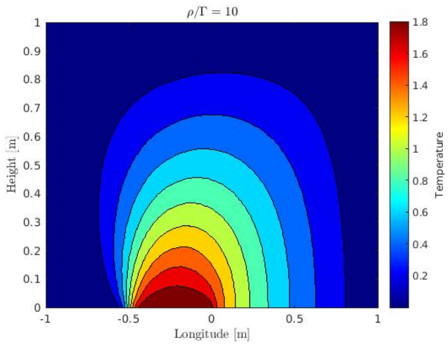
As it can be seen from the previous graphics the source code generated works quite with for all the cases. It can be seen that for a higher Péclet number the results are closer to the numerical ones presented in class. Of course, these results would change depending on the scheme used.

9.2 Results

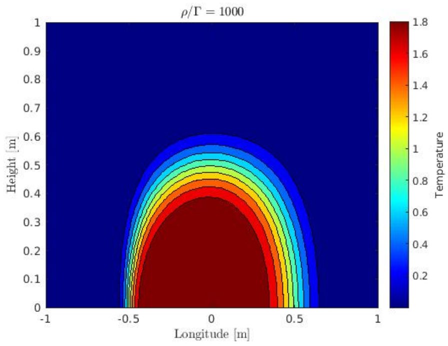
Finally the results for the Smith-Hutton case study are presented. As it is expected the results show a similar behaviour to the previous seen use cases.

It can be clearly seen that, as before, the Péclet number has an influence on the results but as this becomes higher than 1000, the difference between the obtained results is almost none.

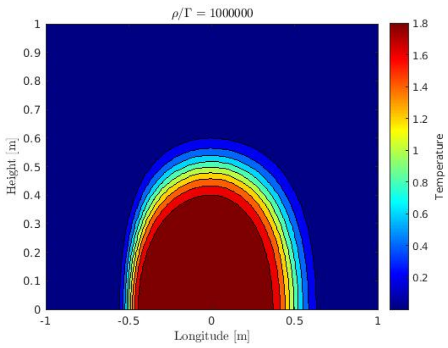
The results obtained for this last case study can be seen in the following figures:



(a) $Pe = 10$



(b) $Pe = 10^3$



(c) $Pe = 10^6$

Figure 10: Temperature field results for the Smith-Hutton case study

10 Computational cost

Lastly, a plot taking into account the computational cost of the different case studies in terms cost iterations and time has been done.

In one hand, it can be clearly seen how the Péclet number, even dough impacts the final results it does not have much and impact on the consumed resources. It is interesting dough, how for small Pe numbers, it does affect a bit. On the other hand, it can be seen how the increase of the number of nodes affects both the computational time and the number of iterations solver needs to do.

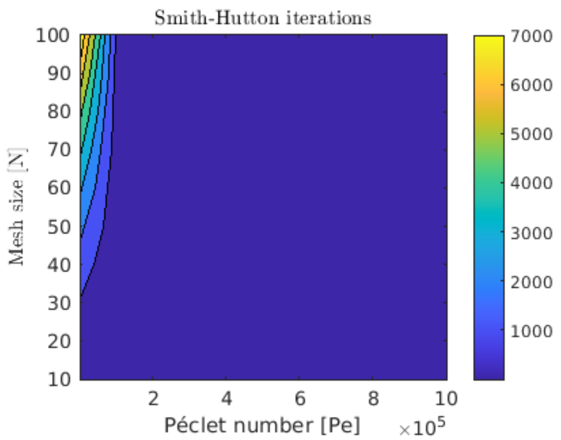


Figure 11: Number of iterations

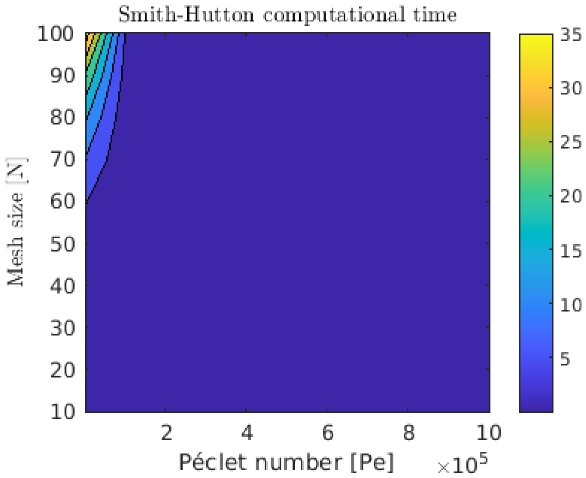


Figure 12: Computational time in terms of Pe and M

References

[1] CTTC. *Numerical resoluition of the convection-diffusion problems*. 202.

[2] Cengel, Y. A. *Heat transfer: a practical approach*, 2nd ed. 2004.

[3] V.Patankar, S. *Numerical Heat Transfer and Fluid Flow*, 1st ed. 1980.

[4] White, F. M. *Fluid Mechanics*, 5th ed.

A Appendix

Equation Terms	Description
Continuity	This equation defines that the variation of mass in the control volume has to be equal to the mass flow through its faces.
$\frac{d\rho}{dt}$	Variation of mass inside the control volume in a differential time.
$\nabla \cdot (\rho \overrightarrow{v})$	Mass flow through the faces of the control volume.
Momentum	This equation shows us that the variation of linear momentum in the control volume plus the momentum flux through the cv faces has to be equal to the sum of the forces that act on the cv.
$\frac{d}{dt}(\rho \overrightarrow{v})$	Represents the variation of linear momentum in the control volume.
$\nabla \cdot (\rho \overrightarrow{v} \overrightarrow{v})$	Represents the momentum flux through the faces of its control volume.
∇p	Pressure gradient acting like an axial force on the faces of the cv.
$\nabla \cdot (\overrightarrow{\tau})$	Total stress tensor. This force acts axially and tangentially on the faces of the control volume. Its value depends on the type of fluid (Newtonian, non-Newtonian...).
$\rho \overrightarrow{g}$	Volumetric force. This force may be a gravitational, electrical, magnetic or electromagnetic.
Energy	Defines that the variation of internal energy and kinetic energy in a control volume plus the flow of their variables must be equal to the work done on the control volume plus the incoming heat flow through the faces of the cv plus the energy of the sources in the control volume.
$\frac{d}{dt}(\rho(u + e_c))$	Represents the variation of the internal and kinetic energy in the cv.
$\nabla \cdot ((u + e_c)\rho \overrightarrow{v})$	Represents the energy flow of these variables through the faces of its volume.
$-\nabla \cdot (\rho \overrightarrow{v})$	Work done by superficial forces like pressure and stress.
$\nabla \cdot \overrightarrow{q}$	Work done by superficial forces like pressure and stress.
$\nabla(\overrightarrow{v} \cdot \overrightarrow{\tau})$	Incoming heat flow through the faces of the control volume.
$\nabla \cdot \overrightarrow{q}$	Represents the work done by the volumetric forces, in this case there is only the gravitational force work.
$\rho \overrightarrow{g} \cdot \overrightarrow{v}$	Work done by the internal forces.