MASTER'S DEGREE IN AERONAUTICAL ENGINEERING

Generic convection-diffusion transport equation

COMPUTATIONAL ENGINEERING

Authors: Ricard Arbat Carandell

Professor: Carlos David Perez Segarra

Escola Superior d'Enginyeria Industrial, Aeroespacial i Audiovisual de Terrassa (ESEIAAT)
Dated: November 21, 2024

Contents

Index of Figures

1 Convection and diffusion

In fluid dynamics, **convection** and **diffusion** describe two mechanisms through which properties such as heat, mass, or momentum are transported within a fluid. Convection refers to the transport of these properties through the bulk motion of the fluid, while diffusion refers to their transport due to molecular motion. Now, some of the most relevant equations and parameters used for modelling this effects will be analyzed:

1.1 Péclet number

The **Péclet number** (Pe) is a dimensionless quantity that characterizes the relative importance of convection versus diffusion in a flow. It is defined as:

$$Pe = \frac{\text{Convective Transport}}{\text{Diffusive Transport}} = \frac{\rho v L}{\Gamma} \tag{1}$$

where L is the characteristic length scale of the problem, and Γ is the diffusion coefficient.

For large Pe, convection dominates, while for small Pe, diffusion dominates. The behavior of numerical schemes can vary significantly depending on the value of Pe, with some schemes performing better for convection-dominated flows and others being more suited to diffusion-dominated flows.

1.2 The convection-diffusion equation

The equation describes the transport of any scalar quantity ϕ (e.g., temperature, concentration, or momentum) due to both convection and diffusion. Starting from the conservation principles and applying the simplifications discussed, we arrive at the generic form of the convection-diffusion equation:

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla \cdot (\rho \mathbf{v} \phi) = \nabla \cdot (\Gamma_\phi \nabla\phi) + S_\phi \tag{2}$$

In this equation:

- ϕ represents a scalar quantity (e.g., temperature, species concentration, or velocity component).
- Γ_ϕ is the diffusion coefficient for the scalar ϕ (e.g., thermal diffusivity for temperature or molecular diffusivity for concentration).
- S_ϕ represents any external source or sink of ϕ (e.g., heat sources, chemical reactions).

The left-hand side of the equation represents unsteady ($\partial(\rho\phi)/\partial t$) and convective ($\nabla \cdot (\rho \mathbf{v}\phi)$) transport. The right-hand side represents diffusive transport ($\nabla \cdot (\Gamma_\phi \nabla\phi)$) and any sources or sinks.

For steady-state problems (i.e., $\partial/\partial t = 0$), the equation simplifies to:

$$\nabla \cdot (\rho \mathbf{v}\phi) = \nabla \cdot (\Gamma_\phi \nabla\phi) + S_\phi \tag{3}$$

1.3 Numerical discretization of the convection-diffusion equation

To solve the convection-diffusion equation numerically, we must discretize the spatial and temporal derivatives, it this case using a finite voluem method (FVM)

In the FVM, the domain is divided into small control volumes (CVs), and the governing equations are integrated over each CV. Integrating the convection-diffusion equation over the control volume yields:

$$\int_{V_p} \frac{\partial(\rho\phi)}{\partial t} dV + \int_{S_p} \mathbf{n} \cdot (\rho \mathbf{v}\phi) dS = \int_{S_p} \mathbf{n} \cdot (\Gamma_\phi \nabla\phi) dS + \int_{V_p} S_\phi dV \tag{4}$$

The integrals represent fluxes of ϕ through the control volume surfaces. The convection and diffusion terms are evaluated at the faces of the control volumes using appropriate numerical schemes. Considering a second order approach for ϕ, the equations can be further developed, yielding:

$$\begin{aligned}\frac{\rho_P\phi_P - \rho_P^0\phi_P^0}{\Delta t} V_P + F_e(\phi_E - \phi_P) - F_w(\phi_W - \phi_P) + F_n(\phi_N - \phi_P) - F_s(\phi_S - \phi_P) \\ = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W) + D_n(\phi_N - \phi_P) - D_s(\phi_P - \phi_S) + S_\phi C + S_\phi P \phi_P\end{aligned}$$

1.4 Resolution schemes

When discretizing the convection and diffusion terms, we use schemes that differ in terms of accuracy and stability. Three common schemes for discretizing the convective fluxes at control volume faces are:

1.4.1 Upwind difference scheme (UDS)

The UDS assumes that the value of ϕ at a control volume face is equal to the value of ϕ at the upstream node. This ensures numerical stability, particularly for high Péclet number flows, but it is only first-order accurate.

$$\phi_e = \begin{cases} \phi_P, & \text{if } F_e > 0 \\ \phi_E, & \text{if } F_e < 0 \end{cases} \tag{5}$$

Here, $F_e = \rho u_e S_e$ is the convective flux across the east face of the control volume.

1.4.2 Central difference scheme (CDS)

The CDS assumes that the value of ϕ at a face is the average of the values at the adjacent nodes. This scheme is second-order accurate, but can become unstable in high Péclet numbers.

$$\phi_e = \frac{\phi_P + \phi_E}{2} \tag{6}$$

1.4.3 Hybrid difference Scheme (HDS)

The HDS is a combination of the UDS and CDS schemes. It uses the CDS for low velocities (or low Péclet numbers) and switches to UDS for high velocities. This offers a balance between stability and accuracy.

1.4.4 Power-law difference scheme (PDS)

The Power-Law Difference Scheme (PDS) is based on the power-law formulation of the convection-diffusion equation. It offers a compromise between the stability of UDS in high convection regimes and the accuracy of CDS in low convection regimes, making it well-suited for flows where both convection and diffusion are significant.

The PDS is given by:

$$\phi_e = \frac{\phi_P}{(1 + 0.5|Pe_e|)} + \frac{\phi_E}{(1 + 0.5|Pe_e|)}\left(1 - \frac{0.5|Pe_e|}{1 + 0.5|Pe_e|}\right) \tag{7}$$

1.5 Generalized discretization equation

The general discretized convection-diffusion equation can be rearranged into a more usable form.

$$a_P\phi_P = a_E\phi_E + a_W\phi_W + a_N\phi_N + a_S\phi_S + b_P \tag{8}$$

Where:

$$a_E = D_e \cdot A(|P_e|) + \max(-F_e, 0)$$
$$a_W = D_w \cdot A(|P_w|) + \max(F_w, 0)$$
$$a_N = D_n \cdot A(|P_n|) + \max(-F_n, 0)$$
$$a_S = D_s \cdot A(|P_s|) + \max(F_s, 0)$$
$$a_P = a_E + a_W + a_N + a_S + \frac{\rho\Delta x\Delta y}{\Delta t}$$
$$b_P = \frac{\rho\Delta x\Delta y}{\Delta t}\phi_P^0 + S_P\Delta x\Delta y$$

In the above terms:

- F represents the convective fluxes across the east, west, north, and south faces, respectively. These are computed as $F = \rho u A$, where A is the area of the face.
- D represents the diffusive fluxes across the corresponding faces. These are computed as $D = \frac{\Gamma A}{d}$, where d is the distance between nodes.
- ϕ are the values of ϕ at the east, west, north, and south neighboring nodes.

The different schemes can be applied by using the equations found in Table I in place of the A functions of Equation 8

Scheme	**Formula for A(|P|)**
CDS	$1 - 0.5\|P\|$
UDS	1
HDS	$\max(0, 1 - 0.5(\|P\|))$
PDS	$\max(0, (1 - 0.5(\|P\|)^5))$

Table I. Numerical schemes available in function of the Péclet number

1.6 Resolution algorithm

1. Input parameters:
   - Physical properties: Velocity, channel size, initial value ϕ, time step Δt...
   - Numerical parameters: Converge criteria Δe, mesh cell number...
   - Other options: Scheme to be used (CDS, HDS, UDS, PDS...), exporting format, file name, storage folder...
2. Initial settings:
   - Mesh building for X, Y and t
   - Initial value of ϕ for t = 0
3. Iteration along the cells of the domain:
   - If fluid cell:
     - Speeds for the cell (u, v)
     - Mass flow terms (F)
     - Péclet number and scheme implementation $(A(|P|))$
     - Evaluation of the equation parameters $(a_p, a_e, a_w, a_n, a_s, b)$
     - Calculation of the next value (ϕ_p) using Gauss - Seidel

- If boundary cell:
    - Set boundary value (ϕ_p)

4. Error with last values. Is $|\phi_{old} - \phi_p < \Delta e|$?
    - Yes. Skip to 5 No. Go to 3 and $\phi_{old} = \phi_p$
5. According to parameters, go back to 2 and repeat for multiple cases of:
    - Schemes
    - Péclet numbers
    - Time step size
    - Mesh refinement
    - Type of flow
6. Exporting data to .csv files
7. Plotting using Matlab, and comparison with reference results

2 Problem definition

2.1 Diagonal flow

The first case encompasses a diagonal flow, as seen in Figure 1. The velocity of the flow is constant at an angle of 45º, and the base speed of the flow (V_0) is set to 1 m/s

$$u = V_0 cos(\theta) \quad v = V_0 sin(\theta)$$

As for the boundary conditions, walls above the diagonal are set to a higher variable $\phi_h = 2$, while the other ones to a lower value $\phi_l = 0$.

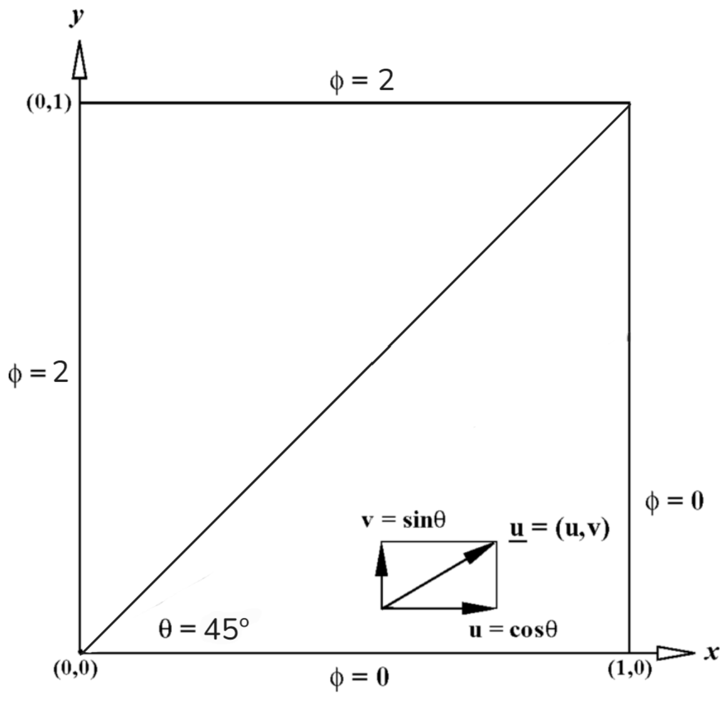


Figure 1. Diagonal flow diagram

2.2 Smith Hutton flow

The second case considers a Smith Hutton constant flow, as seen in Figure 2. The flow comes in from an inlet and follows a velocity field up to the exit. This field is defined as:

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

As for the boundary conditions, there are three different cases:

- **Inlet:** $\phi = 1 + tanh(10(2x + 1))$
- **Walls:** $\phi = 1 + tanh(10)$
- **Outlet:** $\frac{\delta\phi}{\delta y} = 0)$

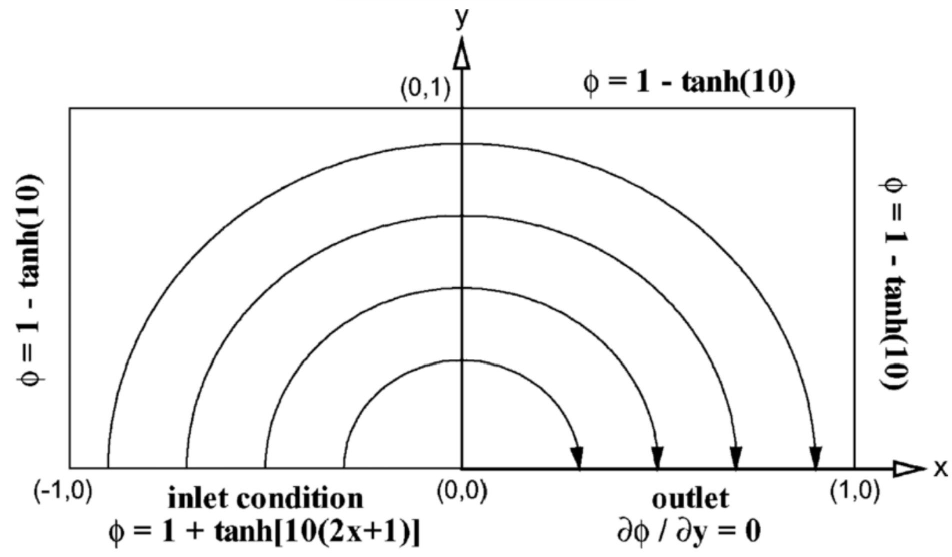


Figure 2. Smith Hutton flow diagram

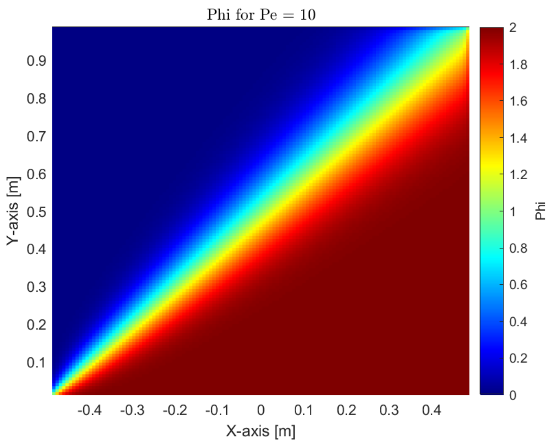
3 Results

3.1 Diagonal flow

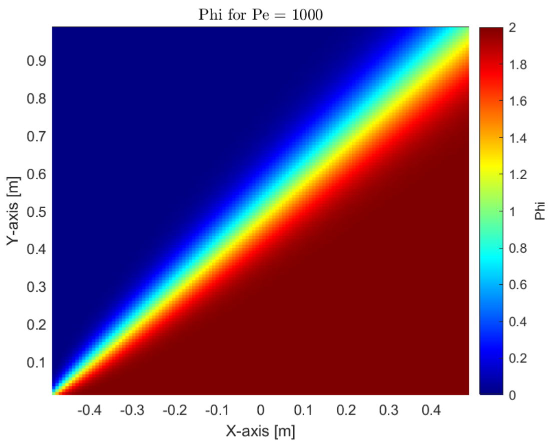
The diagonal flow was obtained as a first simple case, and it was used to check whether the solved worked as expected. The parameters used for the flow were:

- Cells: $M = 128 \;\; N = 128$
- Size: $H = 1m \;\; L = 1m$
- Time step size: $\Delta t = 0.01s$
- Convergence error: $\Delta e = 0.00001$
- Scheme: UDS

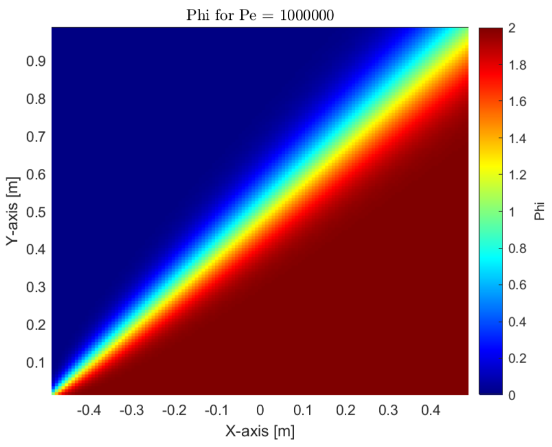
The flow has a clear division between zones of high phi (ϕ_h) and zones with a lower phi (ϕ_l). Also, for lower Péclet numbers, the division is smoother, but as it gets higher, the jump is faster and more abrupt.



(a) Diagonal flow for $Pe = 10$



(b) Diagonal flow for $Pe = 10^3$



(c) Diagonal flow for $Pe = 10^6$

Figure 3. Diagonal flow for multiple Péclet numbers obtained using the UDS scheme

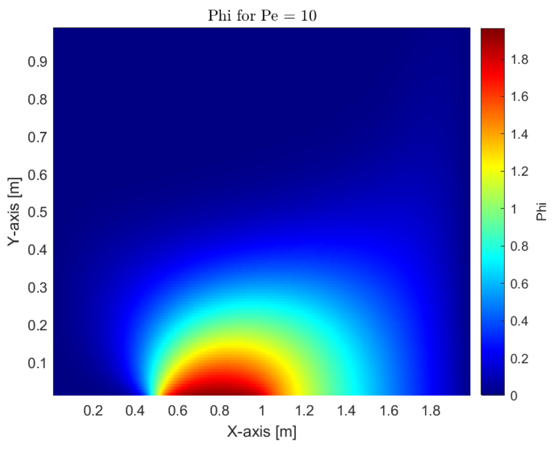
3.2 Smith-Hutton flow

The Smith-Hutton flow was obtained for a case with a relatively high mesh refinement. As it used an HDS scheme, time step size was not very relevant. The parameters used were:

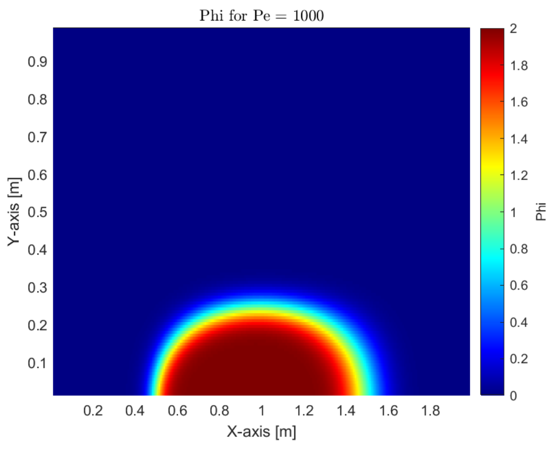
- Cells: $M = 128 \;\; N = 256$
- Size: $H = 1m \;\; L = 2m$
- Time step size: $\Delta t = 0.001s$
- Convergence error: $\Delta e = 0.00001$
- Scheme: HDS

As seen in Figure 4, the resulting 2D maps behave as expected. The value of ϕ defined at the inlet gets transported by the velocity field as expected, reaching the outlet at the end.

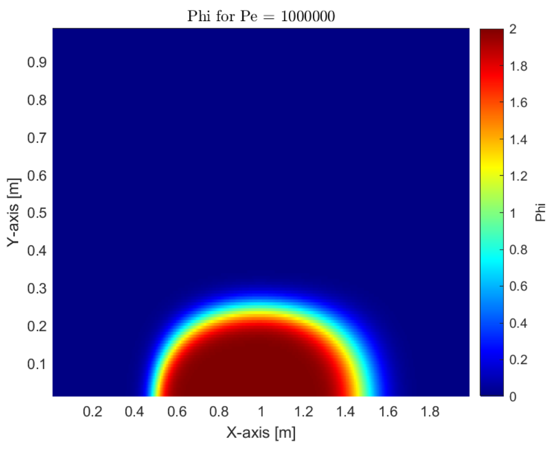
When the Péclet number increases, the change in ϕ becomes more abrupt and fast. This is due to the fact that at higher Péclet numbers, convection is the main transporter of ϕ, while at lower values, diffusion takes more importance.



(a) Smith-Hutton flow for $Pe = 10$



(b) Smith-Hutton flow for $Pe = 10^3$



(c) Smith-Hutton flow for $Pe = 10^6$

Figure 4. Smith-Hutton for multiple Péclet numbers

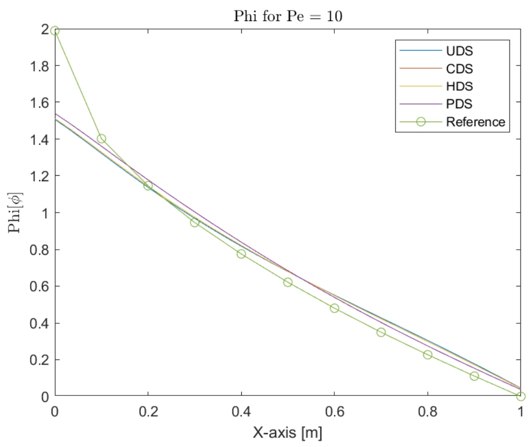
4 Verification

4.1 Schemes

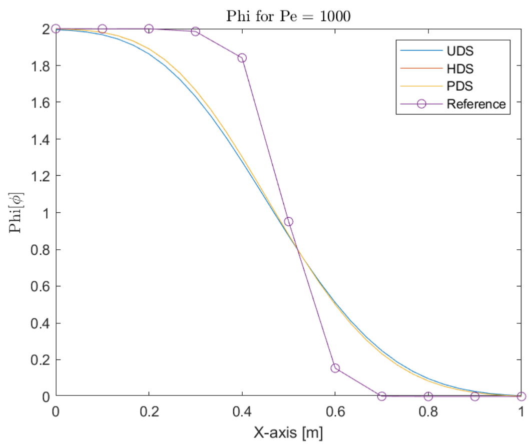
Firstly, the different schemes (UDS, CSD, PDS and HDS) were compared. All of them were compared using some simple parameters:

- Cells: $M = 32 \;\; N = 64$
- Size: $H = 1m \;\; L = 2m$
- Time step size: $\Delta t = 0.01s$
- Convergence error: $\Delta e = 0.0001$

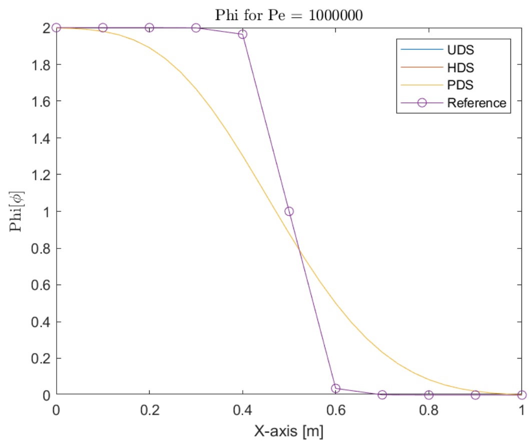
Two main things were observed: Firstly, all the solution schemes gave quite similar results, even though CDS became ustable al higher Pe numbers. And secondly, as the Pe gets higher, the solutions diverge more from the reference result. Both behaviors may mean that more mesh or time refinement are needed.



(a) Parameter (ϕ) at the outlet nodes for a Smith-Hutton flow, $Pe = 10$



(b) Parameter (ϕ) at the outlet nodes for a Smith-Hutton flow, $Pe = 10^3$



(c) Parameter (ϕ) at the outlet nodes for a Smith-Hutton flow, $Pe = 10^6$

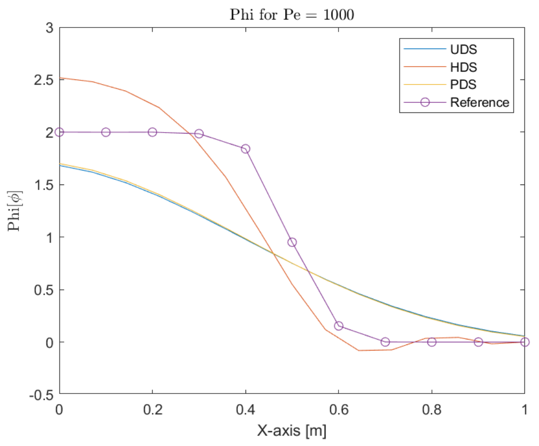
Figure 5. Comparison of ϕ values at the outlet for different schemes and values of Pe

4.2 Convergence to reference results

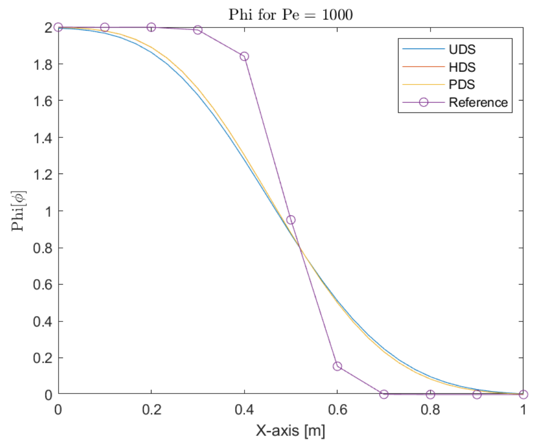
In order to analyze the convergence of the solutions to the reference result, some cases regarding mesh and time delta were studied. The convergence error for the next cases was set to $\Delta e = 0.0001$

4.2.1 Mesh size ($\delta x, \delta y$)

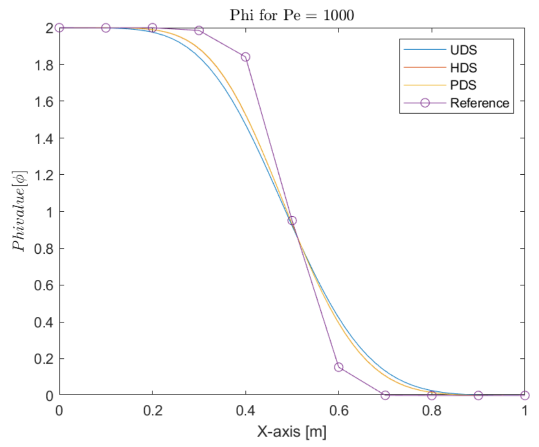
Firstly, the convergence with the mesh refinement was studied. It was seen how (See Figure 6), as the meshes get finer, the numerical approximation gets closer and closer to the reference result. The HDS scheme behaved particularly well, even at low mesh refinements. As it was seen in Figure 5, smaller Pe numbers did not need so much refinement, but as Pe got higher, the difference between the numerical and reference solutions also go higher.



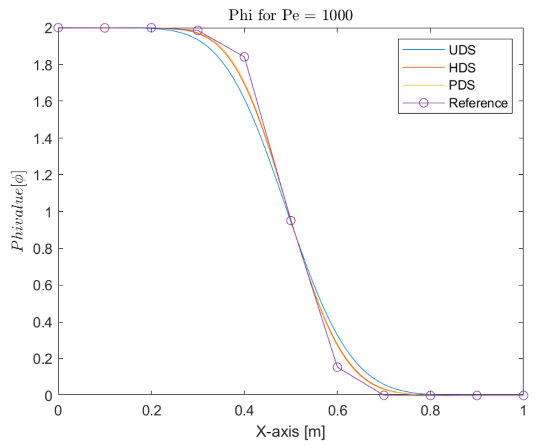
(a) ϕ at the outlet nodes for a Smith-Hutton flow, with $Pe = 10^3$ and $M = 16$ $N = 32$



(b) ϕ at the outlet nodes for a Smith-Hutton flow, with $Pe = 10^3$ and $M = 32$ $N = 64$



(c) ϕ at the outlet nodes for a Smith-Hutton flow, with $Pe = 10^3$ and $M = 64$ $N = 128$



(d) ϕ at the outlet nodes for a Smith-Hutton flow, with $Pe = 10^3$ and $M = 128$ $N = 256$

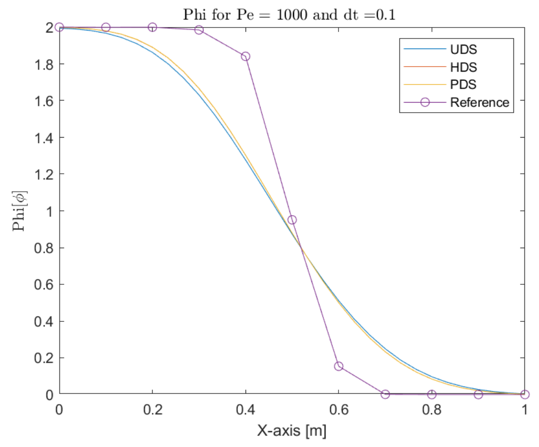
Figure 6. ϕ at the outlet for meshes with different refinement, ranging from M = 16 to M = 128 nodes

As the Péclet number was quite high at 1000, and the numerical parameters used were $\Delta t = 0.01s$ and $\Delta e = 0.0001$, the CDS solution was not stable and diverged. That's why it is not available in the plots. In the next section 4.2.2, this will be analyzed.

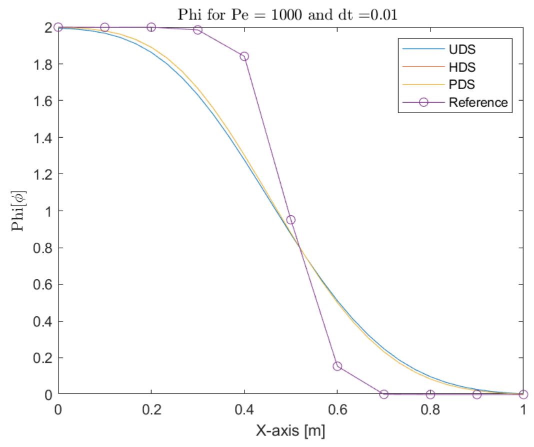
4.2.2 Time step size (Δt)

As for the time step size, some behaviors were also studied. It was observed that the CDS scheme could obtain great results with low mesh refinements, but at the cost of smaller time stepping (See Figure 7).

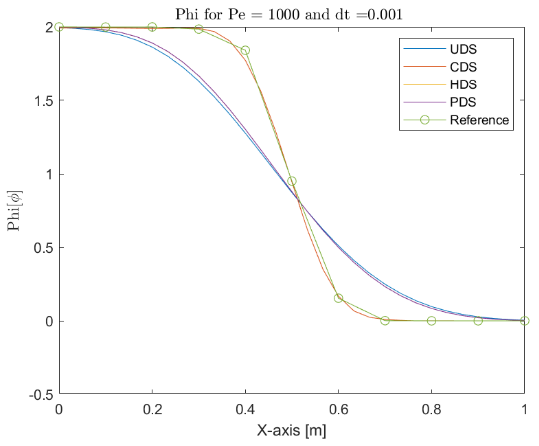
If the time step was too big, for example $\Delta t = 0.01$, the CDS scheme diverged, but as it got smaller, at values of around $\Delta t = 0.001$,even if $M = 32$, the CDS could yield great results, as in Figure 7c



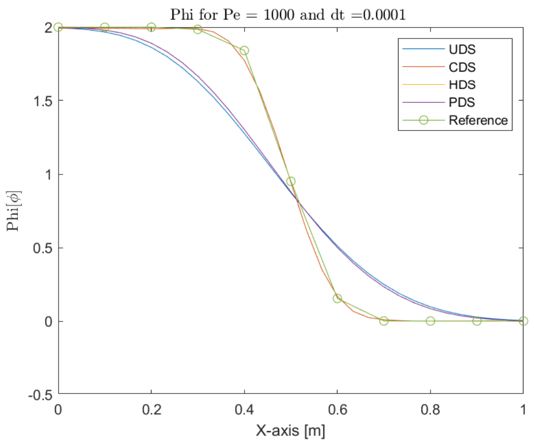
(a) ϕ at the outlet nodes for a Smith-Hutton flow, with $Pe = 10^3$, $M = 32$ and $\Delta t = 0.1$



(b) ϕ at the outlet nodes for a Smith-Hutton flow, with $Pe = 10^3$, $M = 32$ and $\Delta t = 0.01$



(c) ϕ at the outlet nodes for a Smith-Hutton flow, with $Pe = 10^3$, $M = 32$ and $\Delta t = 0.001$



(d) ϕ at the outlet nodes for a Smith-Hutton flow, with $Pe = 10^3$, $M = 32$ and $\Delta t = 0.0001$

Figure 7. ϕ at the outlet for different time refinements, ranging from $\Delta t = 0.1$ to $\Delta t = 0.0001$

References

[1] CTTC. (n.d.). *Course on numerical methods in heat transfer and fluid dynamics: Non-viscous flows*. (accessed: 23-09-2024).

[2] W3Schools. (n.d.). *Learn c++*. https://www.w3schools.com/cpp/ (accessed: 25-09-2024).

[3] Patankar, S. V. (1980). *Numerical heat transfer and fluid flow*. Hemisphere Publishing Corporation.

A C++ Code

The following code has been developed for the report. It allows defining the parameters for either a diagonal or a Smith-Hutton flow, solving it, and then exporting the data for plotting and verification in csv files.

A few Matlab files have also been used in order to plot the data obtained. However, these are not relevant for this report, so they will not be commented, but are available in the *.zip* folder.

A.1 Parameters

The *parameters.cpp* file includes many general parameters used along the code.

```cpp


// Dimensions
int M = 128;                // number of columns
int N = 2 * M;              // number of rows
double H = 1;               // height of the channel
double L = 2 * H;           // length of the channel
const double dx = L / N; // x step
const double dy = L / M; // y step

// Numerical
const int time_steps = 20000;                // number of time steps
const double delta_convergence = 0.00001; // maximum delta for the error
const double initial_phi = 0;                // initial value
double delta_t = 0.001;                      // time step

// Physical
const double rho = 1;    // inlet density
const double S_phi = 0; // source term depenant on phi
const double S_c = 0;    // constant source term

// Diagonal flow
const double u0 = 50;    // inlet velocity for diagonal flow
const double phi_h = 2; // phi value for high side
const double phi_l = 0; // phi value for low side
```

A.2 Meshing

The *mesh.cpp* file contains functions used to build the mesh, set its values and export the data stored in it.

```cpp
// Last update: 2024/10/19
// Author: Ricard Arbat Carandell

// Master in Aerospace Engineering - Computational Engineering
// Universitat Politècnica de Catalunya (UPC) - BarcelonaTech
// Overview: Mesh definition functions

#include <iostream>
#include <vector>
#include <cmath>
#include <fstream>
#include <string>
#include <sstream>
#include "parameters.cpp"
using namespace std;

// node struct
struct node
{
    double x, y, u, v, phi;
};

/**
 * Fills the mesh with nodes as it defines their positions.
 *
 * @param mesh Mesh matrix (vector of vectors) to be filled with Node
    structs
 * @param type Type of problem to solve
 */
void build_mesh(vector<vector<vector<node>>> &mesh, string type)
{
    for (int t = 0; t < time_steps; t++)
    {
        for (int i = 0; i < N; i++)
        {
            for (int j = 0; j < M; j++)
            {
                mesh[t][i][j].x = -1 + (i * dx) + (0.5 * dx);
                mesh[t][i][j].y = (j * dy) + (0.5 * dy);
            }
        }
    }
}

/**
 * Sets the initial density of the mesh nodes.
 * also checks if the node is solid and sets the solid density
 *
 * @param mesh_t Mesh matrix at time t
 * @param variable Value to set
 * @param name Name of the variable to set
 */
void set_mesh_value(vector<vector<node>> &mesh_t, float variable, string
    name)
{
    for (int i = 0; i < N; i++)
    {
        for (int j = 0; j < M; j++)
        {
            if (name == "u")
            {
                mesh_t[i][j].u = variable;
            }
            else if (name == "v")
            {
                mesh_t[i][j].v = variable;
            }
            else if (name == "phi")
            {
                mesh_t[i][j].phi = variable;
            }
        }
    }
}

/**
 * Exports the mesh data to a CSV file
 *
 * @param mesh Mesh matrix at time t
 * @param filename Name of the file to be exported
 * @param folder Folder where the file will be saved
 * @param how_many How many time steps to export. Either "all" or "last".
 **/
void export_data(vector<vector<vector<node>>> &mesh, string filename = "
    output.csv", string folder = "smith_hutton", string how_many = "all")
{

    string header = "s,X,Y,phi,U,V";
    string rows = header + "\n";

    if (how_many == "all")
    {
        for (int t = 0; t < time_steps; t++)
        {
            cout << "Exporting data at time " << t << endl;
            for (int i = 1; i < N - 1; i += 1)
            {
                for (int j = 1; j < M - 1; j += 1)
                {
                    string row = to_string(t * delta_t) + "," + to_string(mesh[t][i][j].x) + "," + to_string(mesh[t][i][j].y) + "," + to_string(mesh[t][i][j].phi) + "," + to_string(mesh[t][i][j].u) + "," + to_string(mesh[t][i][j].v);
                    rows.append(row + "\n");
                }
            }
        }
    }
    else if (how_many == "last")
    {
        int t = time_steps - 1;
        cout << "Exporting data last timestep " << endl;
        for (int i = 1; i < N - 1; i += 1)
        {
            for (int j = 1; j < M - 1; j += 1)
            {
                string row = to_string(t * delta_t) + "," + to_string(mesh[t][i][j].x) + "," + to_string(mesh[t][i][j].y) + "," + to_string(mesh[t][i][j].phi) + "," + to_string(mesh[t][i][j].u) + "," + to_string(mesh[t][i][j].v);
                rows.append(row + "\n");
            }
        }
    }

    string path = folder + "/" + filename;

    ofstream outfile(path);
    outfile << rows << endl;
    outfile.close();
}

/**
 * Exports the mesh data to a CSV file
 *
 * @param mesh Mesh matrix at time t
 * @param scheme Scheme used
 * @param outfile File to write the data
 **/
void export_data_at_outlet(vector<vector<vector<node>>> &mesh, string scheme, ofstream &outfile)
{

```

```cpp
    string rows = scheme + ",";

    int j = 2;
    for (int i = N / 2; i < N - 1; i++)
    {
        string row = to_string(mesh[time_steps - 1][i][j].phi) + ",";
        rows.append(row);
        cout << "x" << mesh[time_steps - 1][i][j].x << " y" << mesh[
    time_steps - 1][i][j].y << " phi" << mesh[time_steps - 1][i][j].phi <<
    endl;
    }
    rows.append("\n");

    outfile << rows << endl;
}

/**
 * Makes a filename with the time and name
 *
 * @param Pe Peclet number
 * @param scheme Scheme used
 * @param name Name of the file
 * @param type Type of problem
 * @param delta_t Time step size
 *
 */
string file_name(double Pe, string scheme, string name, string type, double
    delta_t = 0.001)
{
    std::ostringstream oss;
    if (Pe > 100000.0)
    {
        string Pe_s = "1000000";
        oss << name << "_Pe_" << Pe_s << "_S_" << scheme << "_M_" << M << "
    _type_" << type << "_t_" << delta_t << ".csv";
    }
    else
    {
        oss << name << "_Pe_" << Pe << "_S_" << scheme << "_M_" << M << "
    _type_" << type << "_t_" << delta_t << ".csv";
    }

    std::string var = oss.str();

    return var;
}

```

```
/**
 * Prints the value of phi in the mesh graphically, like a matrix
 *
 * @param values Matrix (Vector of vectors) containing the phi values
 */

void print_phi_matrix(vector<vector<double>> &values)
{
    for (int i = 0; i < N; i++)
    {
        for (int j = 0; j < M; j++)
        {
            cout << values[i][j] << " ";
        }
        cout << endl;
    }
}
```

A.3 Convection-diffusion solver

The *compute_convection_diffusion.cpp* file contains all the algorithms used to compute the simulation.

```
// Last update: 2024/10/19
// Author: Ricard Arbat Carandell

// Master in Aerospace Engineering - Computational Engineering
// Universitat Politècnica de Catalunya (UPC)
// Overview: Convection-diffusion calculations

#define pass (void)0

#include <iostream>
#include <vector>
#include <cmath>
#include <fstream>
#include "mesh.cpp"
using namespace std;

double cds(double P);
double hds(double P);
double eds(double P);
double pds(double P);
double calculate_error(vector<vector<double>> v1, vector<vector<double>> v2)
    ;
void fill_values_at_t(vector<vector<double>> &values, double value);
```

```cpp
void evaluate_time_step_smith_hutton(int t, vector<vector<vector<node>>> &
    mesh, double gamma, double delta_t, string scheme);
void evaluate_time_step_diagonal(int t, vector<vector<vector<node>>> &mesh,
    double gamma, string scheme);

/**
 * Computes iterates the evalueate time step function for each time step.
 * Also selects the type of problem to solve.
 *
 * @param mesh Mesh matrix (vector of vectors)
 * @param gamma Diffusion coefficient
 * @param delta_t Time step size
 * @param scheme Scheme to be used
 * @param type Type of problem
 */

void compute_diffusive_convective(vector<vector<vector<node>>> &mesh, double
     gamma, double delta_t, string scheme, string type)
{

    // Time loop
    for (int t = 1; t < time_steps; t++)
    {
        if (type == "smith-hutton")
        {
            evaluate_time_step_smith_hutton(t, mesh, gamma, delta_t, scheme)
    ;
        }
        else if (type == "diagonal")
        {
            evaluate_time_step_diagonal(t, mesh, gamma, scheme);
        }
    }
}

/**
 * Evaluates the time step of the mesh for the Smith-Hutton problem.
 * Iterates over the mesh and calculates the new phi value for each node
    using the selected scheme.
 *
 * @param t Time instant of the simulation
 * @param mesh Mesh matrix (vector of vectors)
 * @param gamma Diffusion coefficient
 * @param delta_t Time step size
 * @param scheme Scheme to be used
 */
```

```cpp
void evaluate_time_step_smith_hutton(int t, vector<vector<vector<node>>> &
    mesh, double gamma, double delta_t, string scheme)
{
    // Initializing variables for each iteration
    double aE, aW, aN, aS, aP, aP0, b;
    double De, Dw, Dn, Ds;
    double Fe, Fw, Fn, Fs;
    double ue, uw, vn, vs;
    double Pe, Pw, Pn, Ps;
    double Ae, Aw, An, As;
    double phiE, phiW, phiN, phiS;
    double error = 10;
    int cont = 0;

    vector<vector<double>> last_phi(N, vector<double>(M, 0));
    vector<vector<double>> next_phi(N, vector<double>(M, 0));

    // Copy values from last timestep
    for (int i = 0; i < N; i++)
    {
        for (int j = 0; j < M; j++)
        {
            last_phi[i][j] = mesh[t - 1][i][j].phi; // copy phi from
    previous time step
        }
    }

    while (error > delta_convergence)
    {
        for (int i = 0; i < N; i++)
        {
            for (int j = 0; j < M; j++)
            {
                ue = 2 * mesh[t][i][j].y * (1 - ((mesh[t][i][j].x + 0.5 * dx
    ) * (mesh[t][i][j].x + 0.5 * dx)));
                uw = 2 * mesh[t][i][j].y * (1 - ((mesh[t][i][j].x - 0.5 * dx
    ) * (mesh[t][i][j].x - 0.5 * dx)));
                vn = -2 * mesh[t][i][j].x * (1 - ((mesh[t][i][j].y + 0.5 *
    dy) * (mesh[t][i][j].y + 0.5 * dy)));
                vs = -2 * mesh[t][i][j].x * (1 - ((mesh[t][i][j].y - 0.5 *
    dy) * (mesh[t][i][j].y - 0.5 * dy)));

                De = gamma * (dy / dx);
                Dw = gamma * (dy / dx);
                Dn = gamma * (dx / dy);
                Ds = gamma * (dx / dy);

                Fe = rho * dy * ue;
                Fw = rho * dy * uw;
                Fn = rho * dx * vn;
                Fs = rho * dx * vs;

                // Peclet numbers
                Pe = Fe / De;
                Pw = Fw / Dw;
                Pn = Fn / Dn;
                Ps = Fs / Ds;

                // Schemes
                if (scheme == "UDS")
                {
                    Ae = 1;
                    Aw = 1;
                    An = 1;
                    As = 1;
                }
                else if (scheme == "CDS")
                {
                    Ae = cds(Pe);
                    Aw = cds(Pw);
                    An = cds(Pn);
                    As = cds(Ps);
                }
                else if (scheme == "HDS")
                {
                    Ae = hds(Pe);
                    Aw = hds(Pw);
                    An = hds(Pn);
                    As = hds(Ps);
                }
                else if (scheme == "PDS")
                {
                    Ae = pds(Pe);
                    Aw = pds(Pw);
                    An = pds(Pn);
                    As = pds(Ps);
                }
                else if (scheme == "EDS")
                {
                    Ae = eds(Pe);
                    Aw = eds(Pw);
                    An = eds(Pn);
                    As = eds(Ps);
                }
```

```

            aE = De * Ae + max(-Fe, 0.0);
            aW = Dw * Aw + max(Fw, 0.0);
            aN = Dn * An + max(-Fn, 0.0);
            aS = Ds * As + max(Fs, 0.0);

            aP = aE + aW + aN + aS + (rho * dx * dy / delta_t) - (S_phi * dx * dy);

            b = ((rho * dx * dy * mesh[t - 1][i][j].phi) / delta_t) + (S_c * dx * dy);

            if (i == 0)
            {
                next_phi[i][j] = 1 - tanh(10); // bc
            }
            else if (i == N - 1)
            {
                next_phi[i][j] = 1 - tanh(10); // bc
            }
            else if (j == 0)
            {
                if (i < N / 2) // inlet
                {
                    next_phi[i][j] = 1 + tanh(10 * (2 * mesh[t][i][j].x + 1)); // bc
                }
                else // outlet
                {
                    phiE = last_phi[i + 1][j];
                    phiW = last_phi[i - 1][j];
                    phiN = last_phi[i][j + 1];
                    phiS = last_phi[i][j]; // bc
                    next_phi[i][j] = (aE * phiE + aW * phiW + aN * phiN + aS * phiS + b) / aP;
                }
            }
            else if (j == M - 1)
            {
                next_phi[i][j] = 1 - tanh(10); // bc
            }
            else
            {
                phiE = last_phi[i + 1][j];
                phiW = last_phi[i - 1][j];
                phiN = last_phi[i][j + 1];
                phiS = last_phi[i][j - 1];
```

```cpp
                    next_phi[i][j] = (aE * phiE + aW * phiW + aN * phiN + aS * phiS + b) / aP;
                }
            }
        }

        error = calculate_error(next_phi, last_phi);

        if (cont % 100 == 0)
            cout << "Time step: " << t << " Error: " << error << endl;
        cont++;

        for (int i = 0; i < N; i++)
        {
            for (int j = 0; j < M; j++)
            {
                last_phi[i][j] = next_phi[i][j];
            }
        }
    }

    for (int i = 0; i < N; i++)
    {
        for (int j = 0; j < M; j++)
        {
            mesh[t][i][j].phi = next_phi[i][j];
        }
    }
}

/**
 * Evaluates the time step of the mesh for the diagonal flow problem.
 * Iterates over the mesh and calculates the new phi value for each node using the selected scheme.
 *
 * @param t Time instant of the simulation
 * @param mesh Mesh matrix (vector of vectors)
 * @param gamma Diffusion coefficient
 * @param scheme Scheme to be used
 */
void evaluate_time_step_diagonal(int t, vector<vector<vector<node>>> &mesh, double gamma, string scheme)
{
    // Initializing variables for each iteration
    double aE, aW, aN, aS, aP, aP0, b;
    double De, Dw, Dn, Ds;
    double Fe, Fw, Fn, Fs;
    double ue, uw, vn, vs;
    double Pe, Pw, Pn, Ps;
    double Ae, Aw, An, As;
    double phiE, phiW, phiN, phiS;
    double error = 10;
    int cont = 0;

    vector<vector<double>> last_phi(N, vector<double>(M, 0));
    vector<vector<double>> next_phi(N, vector<double>(M, 0));

    // Copy values from last timestep
    for (int i = 0; i < N; i++)
    {
        for (int j = 0; j < M; j++)
        {
            last_phi[i][j] = mesh[t - 1][i][j].phi; // copy phi from
   previous time step
        }
    }

    while (error > delta_convergence)
    {
        for (int i = 0; i < N; i++)
        {
            for (int j = 0; j < M; j++)
            {
                ue = u0 * cos(0.785398);
                uw = u0 * cos(0.785398);
                vn = u0 * sin(0.785398);
                vs = u0 * sin(0.785398);

                De = gamma * (dy / dx);
                Dw = gamma * (dy / dx);
                Dn = gamma * (dx / dy);
                Ds = gamma * (dx / dy);

                Fe = rho * dy * ue;
                Fw = rho * dy * uw;
                Fn = rho * dx * vn;
                Fs = rho * dx * vs;

                // Peclet numbers
                Pe = Fe / De;
                Pw = Fw / Dw;
                Pn = Fn / Dn;
                Ps = Fs / Ds;

                // Schemes
                if (scheme == "UDS")
                {
                    Ae = 1;
                    Aw = 1;
                    An = 1;
                    As = 1;
                }
                else if (scheme == "CDS")
                {
                    Ae = cds(Pe);
                    Aw = cds(Pw);
                    An = cds(Pn);
                    As = cds(Ps);
                }
                else if (scheme == "HDS")
                {
                    Ae = hds(Pe);
                    Aw = hds(Pw);
                    An = hds(Pn);
                    As = hds(Ps);
                }
                else if (scheme == "PDS")
                {
                    Ae = pds(Pe);
                    Aw = pds(Pw);
                    An = pds(Pn);
                    As = pds(Ps);
                }
                else if (scheme == "EDS")
                {
                    Ae = eds(Pe);
                    Aw = eds(Pw);
                    An = eds(Pn);
                    As = eds(Ps);
                }

                aE = De * Ae + max(-Fe, 0.0);
                aW = Dw * Aw + max(Fw, 0.0);
                aN = Dn * An + max(-Fn, 0.0);
                aS = Ds * As + max(Fs, 0.0);

                aP = aE + aW + aN + aS + (rho * dx * dy / delta_t) - (S_phi
 * dx * dy);

                b = ((rho * dx * dy * mesh[t - 1][i][j].phi) / delta_t) + (
S_c * dx * dy);
```

```cpp

                if (i == 0) // Left BC
                {
                    next_phi[i][j] = phi_l;
                }
                else if (i == N - 1) // Right BC
                {
                    next_phi[i][j] = phi_h;
                }
                else if (j == M - 1) // Top BC
                {
                    next_phi[i][j] = phi_l;
                }
                else if (j == 0) // Bottom inlet BC nodes
                {
                    next_phi[i][j] = phi_h;
                }
                else
                {
                    phiE = last_phi[i + 1][j];
                    phiW = last_phi[i - 1][j];
                    phiN = last_phi[i][j + 1];
                    phiS = last_phi[i][j - 1];
                    next_phi[i][j] = (aE * phiE + aW * phiW + aN * phiN + aS * phiS + b) / aP;
                }
            }
        }

        error = calculate_error(next_phi, last_phi);

        if (cont % 100 == 0)
            cout << "Time step: " << t << " Error: " << error << endl;
        cont++;

        for (int i = 0; i < N; i++)
        {
            for (int j = 0; j < M; j++)
            {
                last_phi[i][j] = next_phi[i][j];
            }
        }
    }

    for (int i = 0; i < N; i++)
    {
        for (int j = 0; j < M; j++)
```

```cpp
            {
                mesh[t][i][j].phi = next_phi[i][j];
            }
        }
}

/**
 * Compares two matrices and returns the maximum error between them.
 *
 * @param v1 Matrix (Vector of vectors) to compare
 * @param v2 Matrix (Vector of vectors) to compare
 */
double calculate_error(vector<vector<double>> v1, vector<vector<double>> v2)
{
    double max_error = delta_convergence;
    for (int i = 1; i < v1.size(); i++)
    {
        for (int j = 1; j < v1[i].size(); j++)
        {
            double difference = abs(v1[i][j] - v2[i][j]);
            if (difference > max_error)
            {
                max_error = difference;
            }
        }
    }
    return max_error;
}

/**
 * Fills the initial values of the phi temporal mesh
 *
 * @param values Matrix (Vector of vectors) containing the next stream
   values
 * @param value Value to set for all the nodes
 */
void fill_values_at_t(vector<vector<double>> &values, double value)
{
    for (int i = 0; i < N; i++)
    {
        for (int j = 0; j < M; j++)
        {
            values[i][j] = value;
        }
    }
}

```

```cpp
// Schemes

// Central Difference Scheme
double cds(double P)
{
    return 1 - 0.5 * abs(P);
}

// Hybrid Difference Scheme
double hds(double P)
{
    return max(1 - 0.5 * abs(P), 0.0);
}

// Power Difference Scheme
double pds(double P)
{
    return max(pow(1 - 0.5 * abs(P), 5), 0.0);
}

// Exponential Difference Scheme
double eds(double P)
{
    double val = abs(P) / (exp(abs(P)) - 1) + 0.0000000000001;
    return val;
}
```

A.4 Main

Finally, the main file uses all the defined functions in order to define the parameters, build the mesh, and compute the numerical resolution. It is the entry point of the program, and the one to be executed. A few other files are present in the provided .zip file, each one used to generate different solutions to different cases in a simple way. These codes will not be written here, as they are not relevant enough, but are attached in a *.zip* file:

- *generate_diag_flows.cpp*
- *generate_output_curves.cpp*
- *generate_output_curves_deltat.cpp*
- *generate_smith_hutt_flows.cpp*

And the main file is the following

```cpp
// Last update: 2024/10/19
// Author: Ricard Arbat Carandell

// Master in Aerospace Engineering - Computational Engineering
// Universitat Politècnica de Catalunya (UPC) - BarcelonaTech
// Overview: Main function to solve the convection-diffusion problem.

// Libraries
#include <iostream>
#include <vector>
#include <cmath>
#include <fstream>
#include "compute_diff_conv.cpp"
#include <chrono>
using namespace std;
using namespace std::chrono;

/**
 * Main function of the program. It initializes the mesh, computes the
   stream
 * function and calculates the forces around the cilinder.
 */
int main(void)
{

    double Pe = 1000000;       // peclet number
    double gamma = rho / Pe;   // diffusion coefficient
    string scheme = "PDS";     // scheme to be used
    string type = "diagonal"; // type of problem

    if (type == "smith-hutton")
    {
        N = 2 * M;
    }
    else if (type == "diagonal")
    {
        N = M;
    }

    // Main mesh
    vector<vector<vector<node>>> mesh(time_steps, vector<vector<node>>(N,
   vector<node>(M)));
    build_mesh(mesh, type); // creating the mesh

    set_mesh_value(mesh[0], initial_phi, "phi");

    // Compute stream function
    auto start = high_resolution_clock::now();
    compute_diffusive_convective(mesh, gamma, delta_t, scheme, type); //
   stream solver
    auto stop = high_resolution_clock::now();
    auto duration = duration_cast<microseconds>(stop - start);

    // Export data
    export_data(mesh, file_name(Pe, scheme, "output", type), "output", "last
   ");

    // Print final results
    cout << "### CONVECTION DIFFUSION FLOW RESULTS ###" << endl;
    cout << "Computation time = " << duration.count() / 1000 << "ms" << endl
   ;
    return 0;
}
```