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uFVM v1.0

CFD Academic Tool developed in MATLAB® – User Manual

Computational Mechanics Lab
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2 INTRODUCTION

2.1 USING THE MANUAL

2.1.1 About The Manual

This manual provides an overview about *uFVM* code. The manual describes with sufficient details the structure of the code, the range of applicability and who may use it. The way through which a CFD case is prepared is then described and plenty of tutorials are accordingly provided. In other words, this manual presents a complete set of instructions for the user to follow in order to setup a CFD problem.

2.1.2 Terms of Use

uFVM is an academic CFD tool made for learning purposes. It provides a package of libraries and algorithms that the user can comfortably follow up. Handling, distributing or modifying is fully permissible; the user has the full permission to add any piece of code or modify an existing one.

2.2 ABOUT THE CODE DEVELOPMENT AND AUTHORS

2.2.1 What's *uFVM?*

The name of the code presents an abbreviation letters of the finite volume method (FVM) that the code is based on. The "u" at the beginning of the name points for a fluid flow. The code is developed in Matlab® environment because it is assumed that the majority of interested people are familiar with this environment.

2.2.2 The Place and Time of Development

The code is developed in the computational mechanics lab at the American University of Beirut, Beirut, Lebanon. The development has started in 2003 and was built and updated gradually through years. Lots of versions were made each of them had a different structure but necessarily the same theoretical background.

2.2.3 Developers

The code is a direct accomplishment of the CFD group at the American University of Beirut. The CFD group is a team of professors, graduate and undergraduate students. Their main objective is to build computational knowledge and work on plenty of related topics in both tracks development and application. The team is very familiar with *Ansys Fluent*® and *OpenFOAM*®; they utilize these packages for many purposes. *uFVM* for example was validated in reference to these packages. The group's accomplishments, research topics and published work are posted on their website https://feaweb.aub.edu.lb/research/cfd. The major contributor to the code is

Professor Marwan Darwish[1]. A co-contributor to the code is Professor Fadl Moukalled[2]. The other contributors to the code are Master and PhD students who accomplished their theses and dissertations from the computational mechanics lab at the American University of Beirut.

2.3 Range of Applicability

uFVM works for incompressible fluid flows with any type of mesh (structured and unstructured). For consistency, the code doesn't include any geometry modeling or meshing capabilities. It accepts mesh files of *OpenFOAM* format.

It is worth mentioning that *uFVM* is a solver which solves the conservation equations (transport equations) where the user is able to investigate any physical quantity of interest which is transported by means of a physical phenomenon like convection and diffusion. It is possible also to set any form of an explicit term into the conservation equation like external forces; these are treated as source terms. A transient treatment is also included. The domain usually assumes a fluid flow. However, the code may still apply to solid domains if the user seeks certain transport quantities in a solid, obviously the temperature distribution.

The code may also handle multi-phase flows. The current distributed version of *uFVM* doesn't include compressible and multi-phase solvers as they are still under construction and revision. For further information about the status of multi-phase solver, the user may contact any of the contributors.

It is not the purpose of this code to provide a CFD tool for conducting fluid flow simulations for heavy/complex applications. There are two issues to raise here. First, this code is made for those who are mainly learning CFD and/or interested in CFD code development. This code provides a very useful and helpful means for those people. Second, the user should necessarily realize that Matlab is a highly user friendly language; this makes it very convenient for learning issues much more than it is for conducting real life engineering applications. However, this friendly user specialty had an expense at the computational time; Matlab is slower than other lower level languages.

2.4 A Glance into uFVM's Discretization and Solution Methods

Only pressure-based methods are available in *uFVM* with *SIMPLE* method as the default scheme. The default convection scheme is the *Upwind* scheme, but however, different convection schemes are also available like (*SOU*, *QUICK*, *SMART*, etc.). Gradient computation is based on the first-order Gauss approximation whether it is cell-based or nodal-based. The "ILU" and "SOR" solvers are available along with a multi-grid (AMG) solver which utilizes any of the fixed cycles (V, F, or W Cycle). Under-relaxation factors for any given quantity are treated implicitly in

[1] Professor Darwish has gained his PhD from Brunel University in 1985. His major research topics are computational fluid dynamics, classical fluid mechanics and material sciences. He's currently acting as a full time professor at the American University of Beirut.

[2] Professor Moukalled has gained his PhD from Louisiana University in 1987. His major research topics are compressible flows, computational fluid dynamics, modeling energy systems. He's currently acting as a full time professor at the American University of Beirut.

the equations. All these solution methods and controls are presented in a more detailed framework in later parts of the manual.

3 STRUCTURE OF THE CODE

The *uFVM* directories are distributed into sources, which are the routines that make up the code, and tutorials that include the test cases.

3.1 SOURCE FILES

The source code is available in the 'ufvm/src' directory. It is distributed to different folders, 'fvm' and 'utilities'. 'fvm' contains the finites volume methods, algorithms and solution. 'utilities' contains all auxiliary functions.

3.2 TUTORIALS

There are set of tutorials that allows the user to work with ufvm. These tutorials are classified as basic, incompressible, compressible, multiphase and heatTransfer. Cases that are to be simulated are to be made in OpenFOAM format. OpenFOAM cases include 3 main directories: '0', 'system' and 'constant'. The '0' directory is where initial and boundary conditions are specified. The 'system' directory includes the solution methods, the finite volume schemes and the time and write controls of the simulation. The 'constant' directory includes the mesh files, the fluid properties (transport and/or thermophysical), gravity properties and turbulence properties. For further information, refer to the tutorials.

4 INTRODUCTORY TEST CASE

4.1 MAIN FILE: RUNNING A CASE

The code runs from a main script, usually called 'run'. The 'run' file has to be located in an OpenFOAM case as mentioned earlier. It represents the case study or the problem definition. This is the only file of importance for the user. The main file contains a set of functions that build up the model. However, the user has to add the path of uFVM source files by typing the following command into the command window:

```
addpath(genpath('~location of uFVM~/uFVM/src'));
```

4.2 EXAMPLE

The incompressible 'elbow' example will be presented here.

```
%--------------------------------------------------------------------------
%
%  written by the CFD Group @ AUB, 2017
%  contact us at: cfd@aub.edu.lb
%==========================================================================
% Case Description:
%     In this test case a water flow in an elbow is simulated
%--------------------------------------------------------------------------

% Setup Case
cfdSetupSolverClass('incompressible');

% Read OpenFOAM Files
cfdReadOpenFoamFiles;

% Setup Time Settings
cfdSetupTime;

% Setup Equations
cfdDefineEquation('U', 'ddt(rho*U) + div(rho*U*U) = laplacian(mu*U) + div(mu*transp(grad(U)))
 - grad(p) + rho*g'); % Momentum
cfdDefineEquation('p', 'div(U) = 0'); % Continuity
cfdDefineEquation('T', 'ddt(rho*Cp*T) + div(rho*Cp*U*T) = laplacian(k*T)'); % Energy

% Initialize case
cfdInitializeCase;

% Run case
cfdRunCase;
```

Listing 1 - Run file of the case named 'elbow' in the incompressible tutorials directory

4.2.1 Header

The script starts by few words expressing a header and providing a summary of the case:

```
%--------------------------------------------------------------------------
%
%  written by the CFD Group @ AUB, 2017
%  contact us at: cfd@aub.edu.lb
%==========================================================================
% Case Description:
%     In this test case a water flow in an elbow is simulated
%--------------------------------------------------------------------------
```

4.2.2 Setup Solver Class

The user has to set the class of the application. The application can be one of the following: basic-incompressible-compressible-multiphase-heatTransfer. These are the standard OpenFOAM tutorial classes.

4.2.3 Read OpenFOAM Files

OpenFOAM files are imported at this level to Matlab and stored in a global variable called 'Domain'. In fact, all OpenFOAM input information are stored in a structure called foam within the global Domain variable. The table below presents the settings that the user must or may include in the OpenFOAM files:

Option/Setting Name	*Description*	*Location*
`residualControl`	The equations' tolerances (convergence criteria)	system/fvSolution
`relaxationFactors`	The under-relaxation factors to be applied to the equations	system/fvSolution

`ddtSchemes`	The transient scheme (steady or transient). The options are:
	`steadyState`
	`Euler`
		system/fvSchemes

`divSchemes`	The convection scheme. The options are:
	`Gauss upwind`
	`Gauss linear`
		system/fvSchemes

`startFrom`	This tells the solver from where to start. The options are:
	`firstTime`
	`startTime`
	`latestTime`
		system/controlDict

`startTime`	The initial time of the simulation	system/controlDict
`stopAt`	This tells the solver until when to stop. The options are: `endTime`	system/controlDict
`endTime`	The final time of the simulation	system/controlDict
`deltaT`	The time step of the simulation	system/controlDict
`writeControl`	The criterion that the solver writes the results based on. The options are: `timeStep`	system/controlDict
`writeInterval`	Write results every specified number of time steps (if the	system/controlDict

	`writeControl` is set to `timeStep`)	

4.2.4 Setup Time

The function `cfdSetupTime` sets time controls and other conditions for the simulation. Other conditions of the simulation are related to multiphase flow model which will not be considered in the current uFVM version. The following table presents the valid arguments of the function:

4.2.5 Setup Equations

The user has to define the equations that are to be solved. The equations that are being solved in the above example are described below.

Momentum:

$$\frac{\partial(\rho \boldsymbol{v})}{\partial t} + \nabla.(\rho \boldsymbol{v}\boldsymbol{v}) = \mu \nabla^2 \boldsymbol{v} + \nabla.\{\mu(\nabla \boldsymbol{v})^T\} - \nabla p + \rho \boldsymbol{g}$$

Continuity:

$$\nabla.\boldsymbol{v} = 0$$

Energy:

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla.\left(\rho c_p \boldsymbol{v} T\right) = k \nabla^2 T$$

4.2.6 Initialize Case

The case is initialized after that by evaluating all the fields with their corresponding values on the mesh. For example, the field variables (variables to be solved for), have initial values that are imported from the OpenFOAM '0' directory. The properties are evaluated based on their values dictated by the 'transportProperties' file or 'thermophysicalProperties' file in case of a compressible flow; these are found in the 'constant' directory.

4.2.7 Running the Case

The case is made to run at this level, iterating over the equations until convergence. The convergence criteria can be found in the 'fvSolution' file in the 'system' directory within OpenFOAM folders.

5 READING AND PLOTTING OPENFOAM MESH

When in the case, a user may read the OpenFOAM mesh and visualize it before running the case. The following commands are all what the user needs to do so:

To read the mesh, the function `cfdReadPolyMesh` has to be called. The uFVM will go to the 'constant/polyMesh' directory, read the files there, and store the mesh information in the database. To plot the mesh, the user has to use the function `cfdPlotMesh`; the mesh will then be plotted:

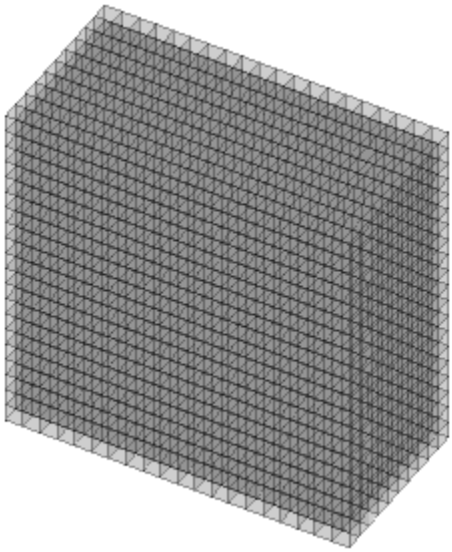


Figure 1 - Plotted mesh

To witness the details of the read mesh, the user has to call for the mesh from the database by writing:

```
mesh = cfdGetMesh
```

The mesh will be printed out such as:

```
mesh =

  struct with fields:

                nodes: [1×4851 struct]
          numberOfNodes: 4851
          caseDirectory: 'constant/polyMesh'
          numberOfFaces: 12800
       numberOfElements: 4000
                faces: [1×12800 struct]
    numberOfInteriorFaces: 11200
             boundaries: [1×3 struct]
      numberOfBoundaries: 3
         numberOfPatches: 3
              elements: [1×4000 struct]
       numberOfBElements: 1600
          numberOfBFaces: 1600
                cconn: {4000×1 cell}
                csize: [4000×1 double]
```

The information printed out above are structures and values that store the quantitative and qualitative details of the mesh. For instance, see the number of elements (numberOfElements: 4000) and the number of patches (numberOfPatches: 3). The information of any element or face can be witnessed by accessing it from the corresponding structure. If I want to see the details of element number 100 in the mesh, I can simply write `mesh.elements(100)` and the output is:

```
>> theMesh.elements(100)


ans =


  struct with fields:


              index: 100
         iNeighbours: [80 99 120 300]
             iFaces: [235 291 294 295 12205 12595]
             iNodes: [104 335 336 105 125 356 357 126]
             volume: 0.1250
           faceSign: [-1 -1 1 1 1 1]
    numberOfNeighbours: 4
          OldVolume: 0.1250
           centroid: [3×1 double]
```

The previous commands can also be applied to faces and nodes. The user may also visualize the elements, faces and patches. In order to plot patch #1 for instance, the function `cfdPlotPatches(1)` has to be called. The output figure is:

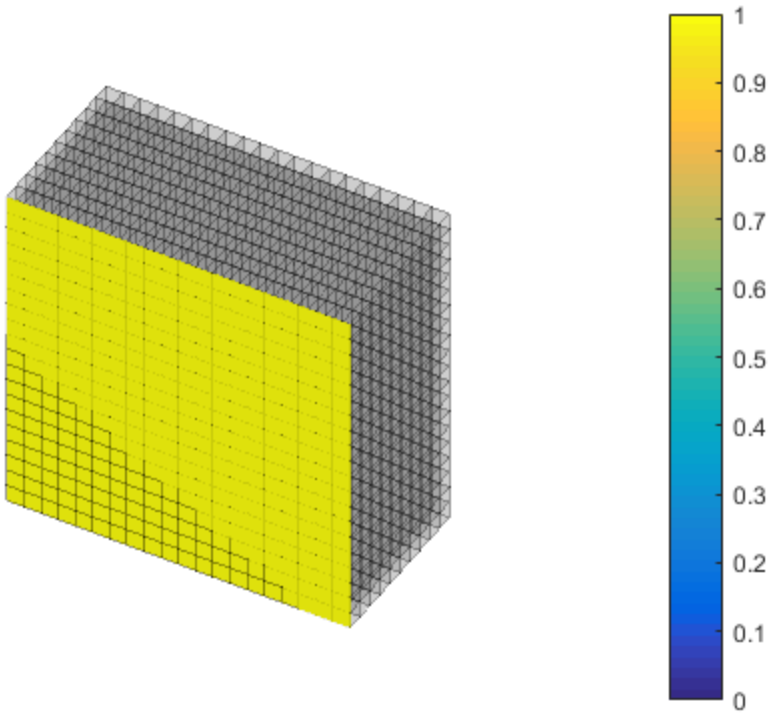


Figure 2 - Plotted mesh and patch number 1

Elements and faces may also be visualized using the functions `cfdPlotElements` and `cfdPlotFaces`. If more than an entity are to be plotted, say 3 entities of indecis 1, 2 and 3, and considering plotting the elements, the user has to call `cfdPlotElements([1 2 3])`. The output figure is:

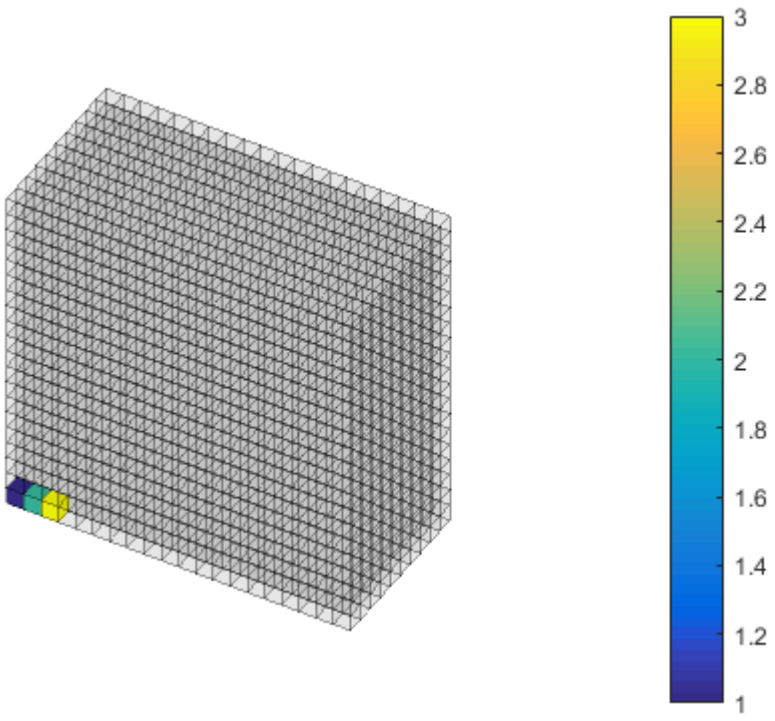


Figure 3 - Visualizing elements 1, 2 and 3

6 AN INTRODUCTORY PRESENTATION OF UFVM FUNCTIONS

6.1 APPLICATION CLASS

Different applications give rise to different ways of treating the fluid flow equations. Thus a user has to set an application class by choosing any of the following applications (basic, incompressible, compressible, heatTransfer and multiphase). It is significantly important to set the right application class because it is the basis of many things inside the code.

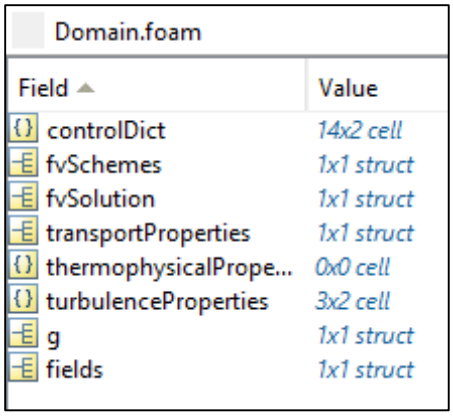
6.2 READING OPENFOAM FILES AND TRANSLATION TO UFVM

As mentioned previously, uFVM cases are prepared in OpenFOAM format. This choice was made because OpenFOAM is a widely used CFD library (C++ based). Preparing an OpenFOAM case is quite straight forward for each application class. Refer to the tutorials and check the way in which each application is being prepared.

uFVM's function `cfdReadOpenFoamFiles` reads all the files that exist in the 3 standard OpenFOAM directories '0', 'constant' and 'system'. It searches for specific entries and blocks within the files and stores them in the uFVM's data base. See the following table for details about the read files:

OpenFOAM Case Directory			
	'system' Directory	fvSolution	block: solvers block: SIMPLE/PISO/ALGORITHM block: relaxationFactors
		fvSchemes	block: ddtSchemes block: divSchemes block: laplcaianSchemes Other Finite Volume Operators
		controlDict	key: startFrom key: startTime key: stopAt key: endTime other control options
	'constant' Directory	polyMesh	boundary points faces owner neighbour Others
		transportProperties/thermophysicalProperties	Collect all properties and their attributes (values, dimensions, models, expressions)
		turbulenceProperties	key: simulationType i.e. RAS key: RASModel key: turbulence key: printCoeffs
		g	Collect gravitational acceleration vale i.e. (0 0 -9.8)
	'0' Directory	U	class internalField boundaryField
		p	class internalField boundaryField
		T	class internalField boundaryField
		Other fields	

The above FOAM details are imported and stored in the data base 'Domain' under the structure 'foam' as such:



6.3 Fixing Time Settings

Of the imported control settings, the time controls which exist in the controlDict structure in the global Domain variable, are stored again in a more useful way in another structure called time.

The structure 'time' contains the following info for the arbitrary case of elbow:

```
>> Domain.time


ans =


  struct with fields:


    startFrom: 'latestTime'
    startTime: 0
      stopAt: 'endTime'
    endTime: 10000
     deltaT: 10
        fdt: 1.0000e+09
       type: 'Transient'
```

The above settings will be used later on to set the start and end of the time loop or convergence loop. If the case is transient, 'deltaT' in the above structure is the time step.

6.4 Interpreting the Model/Equations

The equations in uFVM are interpreted in such a way that each term of the equation has its own attributes. Generally, any conservation equation has the following form:

$$\underbrace{\frac{\partial(\rho\phi)}{\partial t}}_{Transient} + \underbrace{\nabla.(\rho\boldsymbol{v}\phi)}_{Convection} = \underbrace{\nabla.\left(\Gamma^{\phi}\nabla\phi\right)}_{Diffusion} + \underbrace{Q^{\phi}}_{Source}$$

Note: The diffusion term $\nabla.\left(\Gamma^{\phi}\nabla\phi\right)$ can only be written as $\Gamma\nabla^2\phi$ when the diffusion coefficient Γ is constant. However, when implementing the diffusion term in uFVM, it is always written as laplacian(tau*phi) whether Γ is constant or not.

The general conservation equation above is expressed in uFVM as follows:

```
cfdDefineEquation('phi', 'ddt(rho*phi) + div(rho*U*phi) = laplacian(tau*phi) + Q');
```

Q in the above implementation has to be an explicit expression that includes fields and/or properties. Inside uFVM, each of the above terms is interpreted in a different way. Each term consists of an explicit part and an implicit one; the explicit part is the part which holds the previous iteration value, and the implicit part is kept as an unknown to be assembled with other implicit parts of other terms in a global matrix. The explicit part is roughly all the parameters that are multiplied with ϕ and the implicit part is ϕ. In the case of a general conservation equation, the explicit part of the transient term $\frac{\partial(\rho\phi)}{\partial t}$ is ρ and the implicit part is ϕ. In addition, the explicit part of the transient term, is called the ***rho*** field. For the convection and diffusion terms, the explicit parts are $\rho\boldsymbol{v}$ and Γ respectively, and the names of the latter explicit fields are the ***psi*** field and the ***gamma*** field respectively. The source term is treated explicitly; it is evaluated based on available field values.

The table below summarizes the treatment of the terms of a general conservation equation:

$\frac{\partial(\rho\phi)}{\partial t}$	The term type: Transient Term
	the ***rho*** field: ρ
	the variable field: ϕ
$\nabla.(\rho\boldsymbol{v}\phi)$	The term type: Convection Term
	the ***psi*** field: $\rho\boldsymbol{v}$
	the variable field: ϕ
$\nabla.(\Gamma^{\phi}\nabla\phi)$	The term type: DiffusionTerm
	the ***gamma*** field: Γ^{ϕ}
	the variable name: ϕ
Q^{ϕ}	The term type: Source term

Example1:

Take the momentum equation in the elbow case as an example:

$$\frac{\partial(\rho \boldsymbol{v})}{\partial t} + \nabla.(\rho \boldsymbol{v}\boldsymbol{v}) = \mu\nabla^2\boldsymbol{v} + \nabla.\{\mu(\nabla \boldsymbol{v})^T\} - \nabla p + \rho \boldsymbol{g}$$

It is written in uFVM in the following form:

```
'ddt(rho*U) + div(rho*U*U) = laplacian(mu*U) + div(mu*transp(grad(U))) - grad(p) + rho*g'
```

The momentum equation above includes 6 terms, each of them is interpreted in uFVM as shown here:

ddt(rho*U)	The term type: Transient Term
	Finite Volume Operation: Implicit
	the rho field: rho
	the variable field: U
	term sign: 1
div(rho*U*U)	The term type: Convection Term
	Finite Volume Operation: Implicit
	the psi field: rho*U
	the variable field: U
	term sign: 1
laplacian(mu*U)	The term type: Stress Term
	Finite Volume Operation: Implicit
	the gamma field: mu
	the variable name: U
	term sign = -1
div(mu*transp(grad(U)))	The term type: Source term
	Finite Volume Operation: Explicit
	explicit operators available: grad
	term sign: -1
grad(p)	The term type: Source term
	Finite Volume Operation: Explicit
	explicit operators available: grad
	term sign: 1
rho*g	The term type: Source term
	Finite Volume Operation: Explicit
	explicit operators available: none
	term sign: -1

Example2:

Take the Energy equation in the elbow case as another example:

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla.\left(\rho c_p \boldsymbol{v} T\right) = k\nabla^2 T$$

It is written in uFVM in the following form:

```
'ddt(rho*Cp*T) + div(rho*Cp*U*T) = laplacian(k*T)'
```

The Energy equation above includes 3 terms, each of them is interpreted in uFVM as shown here:

ddt(rho*Cp*T)	The term type: Transient Term
	Finite Volume Operation: Implicit
	the rho field: rho*Cp
	the variable field: T
	term sign: 1
div(rho*Cp*U*T)	The term type: Convection Term
	Finite Volume Operation: Implicit
	the psi field: rho*Cp*U
	the variable field: T
	term sign: 1
laplacian(k*T)	The term type: Stress Term
	Finite Volume Operation: Implicit
	the gamma field: k
	the variable name: T
	term sign = -1

However, a special case arises for the continuity equation which is usually called also the pressure equation 'p'. The 'p' equation is treated in a different way. The pressure equation for an incompressible application class is the same for any fluid flow problem within the incompressible category. Thus, the user may ignore the pressure equation expression keeping only the equation name ('p'). The reason that the pressure equation expression is included in the Matlab listing above and we are repeating it here is just for showing the exact models that this code is solving:

```
cfdDefineEquation('p', 'div(U) = 0');
```

While it is sufficient to write:

```
cfdDefineEquation('p');
```

Automatically, all the terms of the continuity equation are treated in a single term assembly process, this term is called 'mdot'. For incompressible fluid flows, the continuity equation stated above is theoretically converted into another equation called the pressure equation, and that's why the name 'p' corresponds to the continuity equation.

A summary of how the pressure equation is derived from the continuity equation is presented here:

The continuity equation for an incompressible flow:

$$\nabla . \boldsymbol{v} = \mathbf{0}$$

$$\rightarrow \sum_{f\sim nb(C)} \dot{m}_f = 0$$

Dividing $\dot{m}_f$ into a predicted and correction components:

$$\dot{m}_f = \dot{m}_f^* + \dot{m}_f'$$

So,

$$\sum_{f\sim nb(C)} \dot{m}_f' + \sum_{f\sim nb(C)} \dot{m}_f^* = 0$$

The Rhie-Chow interpolation for $\dot{m}_f^*$ is

$$\dot{m}_f^* = \rho_f \overline{\boldsymbol{v}_f^*}.\boldsymbol{S}_f - \rho_f \overline{\boldsymbol{D}_f^{\boldsymbol{v}}} \left(\nabla p_f^{(n)} - \overline{\nabla p_f^{(n)}}\right).\boldsymbol{S}_f$$

and for $\dot{m}_f'$ is

$$\dot{m}_f' = -\rho_f \overline{\boldsymbol{D}_f^{\boldsymbol{v}}} \nabla p_f'.\boldsymbol{S}_f$$

Therefore, the equation of the incompressible pressure equation is:

$$\underbrace{\sum_{f\sim nb(C)} -\rho_f \overline{\boldsymbol{D}_f^{\boldsymbol{v}}} (\nabla p'_f).S_f + \sum_{f\sim nb(C)} \dot{m}_f^*}_{mdot\_f} = 0$$

For a compressible continuity equation, the resulting pressure equation is a follows (you may find the proof in the book):

$$\underbrace{\frac{V_C C_\rho}{\Delta t} p_C' + \sum_{f\sim nb(C)} C_{\rho,f} \left(\frac{\dot{m}_f^*}{\rho_f^*}\right) p_f' + \sum_{f\sim nb(C)} -\rho_f \overline{\boldsymbol{D}_f^{\boldsymbol{v}}} (\nabla p'_f).S_f + \frac{(\rho_C^* - \rho_C^\circ)}{\Delta t} + \sum_{f\sim nb(C)} \dot{m}_f^*}_{mdot\_f} = 0$$

6.5 RUNNING THE CASE

6.5.1 Time Loop/Convergence Loop

The time loop and the convergence loop are located in the `cfdRunCase` where the time settings are utilized. The following listing shows the time and convergence loops for a transient simulation:

```
time = cfdGetTime;
startTime = time.startTime;
endTime = time.endTime;
deltaT = time.deltaT;

% Time Loop: Loop until the final time
timeIter = 1;
cumulativeIter = 1;
for t=startTime:deltaT:endTime
    % Time settings
    currentTime = t + deltaT;
    cfdSetCurrentTime(currentTime);

    % Update previous time step fields
    cfdTransientUpdate;

    cfdPrintCurrentTime(currentTime);

    % Convergence Loop: Loop until convergence for the current time step
    for iter=1:20
        cfdPrintIteration(cumulativeIter);
        cfdPrintResidualsHeader;
        %
        cfdUpdateFields;
        %
        for iEquation=1:theNumberOfEquations
            % Assemble the current equation and correct it
            [rmsResidual, maxResidual, lsResBefore, lsResAfter] = cfdAssembleAndCorrectEquation(theEquationNames{iEquation});

            % Print the equation residuals
            cfdPrintResiduals(cfdGetBaseName(theEquationNames{iEquation}),rmsResidual,maxResidual,lsResBefore,lsResAfter);

            % If multigrid solver is assigned, print the AMG solver
            % settings
            theEquation = cfdGetModel(theEquationNames{iEquation});
            isMultigrid = theEquation.multigrid.isActive;
            if isMultigrid
                cfdPrintLinearSolver(theEquationNames{iEquation});
                if iEquation<theNumberOfEquations
                    cfdPrintResidualsHeader;
                end
            end

            % Store RMS residuals to check for convergence later on
            convergenceCriterion{iEquation}(1:length(maxResidual)) = rmsResidual;
        end
        fprintf('|=============================================================================|\n');
        cfdPrintCPUTime;

        cfdPlotRealTimeResiduals(cumulativeIter);

        % Check for convergence at each iteration at the current time
        % step
        isConverged = cfdCheckConvergence(convergenceCriterion);
        if isConverged
            fprintf('Solution is converged!\n')
            break;
        end
        cumulativeIter = cumulativeIter + 1;
    end
    cfdWriteResults(timeIter, currentTime);
    timeIter = timeIter + 1;
end
```

Listing 2 – Time loop

Note that the time settings startTime, endTime and deltaT are retrieved from the structure called ‘time’ in the data base.

6.5.2 Assembling Equation Terms

The main function which includes all the finite volume methods (assembling equation terms, solving and correcting) is `cfdAssembleAndCorrectEquation`. The aim of discretizing is to assemble the algebraic coefficients and build the algebraic system of the model equation:

$$a_C \phi_C + \sum_{F \sim NB(C)} a_F \phi_F = b_C$$

And after that, the function proceeds to solve a set of algebraic system $A\phi = b$ which yields a solution of the system.

The following listing shows the main content of this function:

```
    for iCorrector=1:nCorrectors
        % Assemble Equation
        [rmsResidual(iComponent), maxResidual(iComponent)] = cfdAssembleEquation(theEquationName,iComponent);

        % Solve Equation
        [initialResidual(iComponent),finalResidual(iComponent)] = cfdSolveEquation(theEquationName);

        % Correct Equation
        cfdCorrectEquation(theEquationName,iComponent);
    end

    % Store rms residual in the equation model
    cfdStoreResiduals(theEquationName, iComponent, rmsResidual(iComponent));
end
```

Listing 3 - Assembling, solving, correcting the equation and storing its residuals

Starting with assembling the equation, the function `cfdAssembleEquation` executes the following commands:

```
% Assemble Equation Terms
[rmsResidual, maxResidual] = cfdAssembleEquationTerms(theEquationName,iComponent);

% Post Assemble Equation
cfdPostAssembleEquation(theEquationName,iComponent);
```

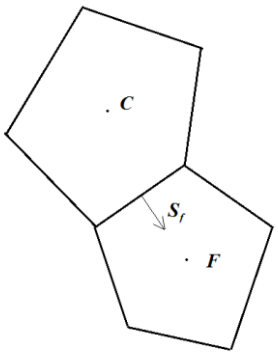
Listing 4 - Assembling equation terms and post assembling

The function `cfdAssembleEquationTerms` is in fact the function that includes the term assembly and it is shown in the listing below, while the function `cfdPostAssembleEquation` includes some methods that are done after assembling.

```
for iTerm = 1:theNumberOfTerms
    theTerm = theEquation.terms{iTerm};
    if strcmp(theTerm.name,'Transient')
        cfdAssembleTransientTerm(theEquationName,theTerm,iComponent);
    elseif strcmp(theTerm.name,'Convection')
        cfdAssembleConvectionTerm(theEquationName,theTerm,iComponent);
    elseif strcmp(theTerm.name,'Diffusion')
        cfdAssembleDiffusionTerm(theEquationName,theTerm);
    elseif strcmp(theTerm.name,'Stress')
        cfdAssembleStressTerm(theEquationName,theTerm,iComponent);
    elseif strcmp(theTerm.name,'mdot_f')
        cfdAssembleMdotTerm(theEquationName,theTerm);
    elseif strcmp(theTerm.name,'Source')
        cfdAssembleSourceTerm(theEquationName,theTerm,iComponent);
    elseif strcmp(theTerm.name,'Implicit Source')
        cfdAssembleSourceTerm(theEquationName,theTerm,iComponent);
    else
        error('\n%s\n',[theTerm.name,' term is not defined']);
    end
end
```

Listing 5 - Assembling of the terms in `cfdAssembleEquationTerms`

The assembling of the terms is made according to the finite volume method. The finite volume method states that the conservation equation is integrated on an element C of volume V_C. The figure below shows an element C with neighboring element F:



The general conservation equation is:

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla.(\rho\boldsymbol{v}\phi) = \nabla.\left(\Gamma^{\phi}\nabla\phi\right) + Q^{\phi}$$

Integrating the equation over the volume of element C:

$$\rightarrow \int_{V_C} \frac{\partial(\rho\phi)}{\partial t} dV + \int_{V_C} \nabla.(\rho\boldsymbol{v}\phi) = \int_{V_C} \nabla.\left(\Gamma^{\phi}\nabla\phi\right) dV + \int_{V_C} Q^{\phi}\, dV$$

Applying finite volume time discretization approach for transient term and Greens' theorem to convection and diffusion terms:

$$\rightarrow \frac{\rho_C\phi_C - \rho_C^{\circ}\phi_C^{\circ}}{\Delta t} V_C + \sum_{f\sim nb(C)} \left(\rho_f \boldsymbol{v}_f.\boldsymbol{S}_f\phi_f\right) = \sum_{f\sim nb(C)} \left(\Gamma_f^{\phi}\nabla\phi_f.\boldsymbol{S}_f\right) + Q_C^{\phi}V_C$$

The coefficient $\rho_f\boldsymbol{v}_f.\boldsymbol{S}_f$ in the second term (convection term) is referred to as ψ_f; this is mentioned earlier. So, the equation is now:

$$\frac{\rho_C\phi_C - \rho_C^{\circ}\phi_C^{\circ}}{\Delta t} V_C + \sum_{f\sim nb(C)} \left(\psi_f\phi_f\right) = \sum_{f\sim nb(C)} \left(\Gamma_f^{\phi}\nabla\phi_f.\boldsymbol{S}_f\right) + Q_C^{\phi}V_C$$

For each element, this is the semi-discretized equation. The terms above are now distributed into element and face fluxes.

6.5.2.1 Transient Term

The semi-discretized transient term $\frac{\rho_C\phi_C - \rho_C^{\circ}\phi_C^{\circ}}{\Delta t} V_C$ is a contribution from the element itself but not from the surrounding (through faces) like the convection and diffusion terms, so it is added to the element flux such as follows:

$$fluxC = \frac{\rho_C}{\Delta t} V_C$$

$$fluxC^{\circ} = -\frac{\rho_C^{\circ}}{\Delta t} V_C$$

$$fluxV = 0$$

$$fluxT = fluxC\phi_C + fluxC^{\circ}\phi_C^{\circ} + fluxV$$

In uFVM, the function `cfdAssembleTransientTermEuler` calculates the above fluxes as shown in the listing below:

```
theFluxes.FLUXCE    =   theTerm.sign * vol .* rho / deltaT;
theFluxes.FLUXCEOLD = - theTerm.sign * vol .* rho_old / deltaT;
theFluxes.FLUXTE    =   theFluxes.FLUXCE .* phi' + theFluxes.FLUXCEOLD .* phi_old';
```

Listing 6 - Assmebling transient term based on Euler's method

6.5.2.2 Convection Term

The face fluxes of the convection term $\sum_{f\sim NB(C)}(\psi_f \phi_f)$ based on a first order upwind scheme are calculated as follows:

$$fluxCf = \|\psi_f, 0\|$$

$$fluxFf = -\|-\psi_f, 0\|$$

$$fluxVf = 0$$

$$fluxTf = fluxCf\phi_C + fluxFf\phi_F + fluxVf$$

The listing below is retrieved from `cfdAssembleConvectionTerm`:

```
theFluxes.FLUXC1f(iFaces,1) =   theTerm.sign * max(psi,0);
theFluxes.FLUXC2f(iFaces,1) = - theTerm.sign * max(-psi,0);
theFluxes.FLUXVf(iFaces,1) =    0;
theFluxes.FLUXTf(iFaces,1) = theFluxes.FLUXC1f(iFaces) .* phi(iOwners) + theFluxes.FLUXC2f(iFaces) .*
phi(iNeighbours) + theFluxes.FLUXVf(iFaces);
```

Listing 7 - Calculating face fluxes from the convection term contribution. It is retrieved from the function

The above assembly is based on a first order upwind convection scheme. If a higher order scheme is required and additional non-linear face flux arises. For a second order upwind convection scheme, we have in addition to the above fluxes:

$$fluxVf = (2\nabla\phi_C - \nabla\phi_f).\boldsymbol{d}_{CF}$$

A glance to the implementation is shown here:

```
rC = [theMesh.elements(iUpwind).centroid]';
rf = [theMesh.faces(iFaces).centroid]';
rCf = rf - rC;

corr = psi .* dot(2*phiGradC' - phiGradf(iUpwind, :)',rCf')';

theFluxes.FLUXTf(iFaces) = theFluxes.FLUXTf(iFaces) +  corr;
```

Listing 8 - Assembling of the correction term for higher order convection scheme (SOU)

6.5.2.3 Diffusion Term

The face fluxes of the diffusion term $\sum_{f\sim nb(C)}\left(\Gamma_f^{\phi}\nabla\phi_f.\boldsymbol{S}_f\right)$ are calculated as follows. The linear face fluxes are:

$$fluxCf = -\Gamma_f^{\phi} gDiff_f$$

$$fluxFf = \Gamma_f^{\phi} gDiff_f$$

$gDiff_f$ is the geometric difference at the face; it is calculated as:

$$gDiff_f = \frac{E_f}{\boldsymbol{d}_{CF}}$$

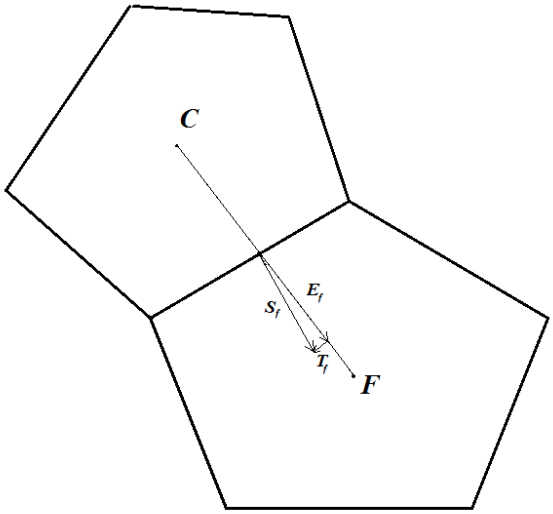
Where E_f is the norm of the vector $\boldsymbol{E}_f$, which is the non-orthogonal component of $\boldsymbol{S}_f$:

$$\boldsymbol{S}_f = \boldsymbol{E}_f + \boldsymbol{T}_f$$

The non-linear face flux is:

$$fluxVf = \Gamma_f^{\phi} \nabla\phi_f . \boldsymbol{T}_f$$

The above non-linear face flux includes the previous iteration value of $\nabla\phi_f$ as well as the non-orthogonal component of the face surface vector $\boldsymbol{S}_f$ which is shown in the figure below:



The total flux is then:

$$fluxTf = fluxCf\phi_C + fluxFf\phi_F + fluxVf$$

The following piece of code is retrieved from the function `cfdAssembleDiffusionTerm`:

```
theFluxes.FLUXC1f(iFaces,1) = - theTerm.sign * gamma .* gDiff_f;
theFluxes.FLUXC2f(iFaces,1) =   theTerm.sign * gamma .* gDiff_f;
theFluxes.FLUXVf(iFaces,1)  =   theTerm.sign * gamma .* dot(grad_f(:,:)',Tf(:,:)')';
theFluxes.FLUXTf(iFaces,1)  =   theFluxes.FLUXC1f(iFaces) .* phi(iOwners) + theFluxes.FLUXC2f(iFaces) .*
phi(iNeighbours) + theFluxes.FLUXVf(iFaces);
```

Listing 9 - Assembling diffusion term to face fluxes

6.5.2.4 Source Term

The source terms are all terms that are to be treated explicitly in the equation assembly. Any source term is discretized and assembled as an element flux as follows:

$$fluxV = Q_C^{\phi} V_C$$

$$fluxT = fluxV$$

It is worth mentioning that in uFVM, source terms are either recognized as standard source terms or non-standard source terms. Of the standard source terms are gradients of equation fields ($\nabla \boldsymbol{v}, \nabla p, \nabla T, etc$). In the momentum equation for example, there's a pressure gradient term ∇p. Instead of calculating the pressure gradient to assemble it, it is available in the data base. So it is only called from the data base; this saves some time.

The non-standard source terms are evaluated directly as they appear in the equation. Of the non-standard terms are:

$\nabla.\{\mu(\nabla \boldsymbol{v})^T\}$	The second part of shear stress term. It appears in the momentum equation
$-\frac{2}{3}\nabla(\mu \nabla. \boldsymbol{v})$	The third part of the shear stress term which includes the bulk viscosity for compressible flows. It appears in the momentum equation.
$\rho \boldsymbol{g}$	A body force (weight of fluid) which appears in the momentum equation

The following listing shows the assembly of a non-standard term retrieved from the function `cfdAssembleSourceTerm`:

```
% If source term is not standard
S = cfdEvaluateNonstandardSourceTerm(theTerm, iComponent);

% Assemble Source Term as element flux
theFluxes.FLUXTE = theTerm.sign * S .* volume;
cfdAssembleIntoGlobalMatrixElementFluxes(theEquationName,theFluxes,iComponent);
```

Listing 10 - Assembling non-standard source term

6.5.2.5 'mdot_f' Term

The pressure correction equation is treated within a single term called 'mdot_f' term. The incompressible pressure equation

$$\underbrace{\sum_{f\sim nb(C)} -\rho_f \overline{\boldsymbol{D}_f^{\boldsymbol{v}}} (\nabla p'_f).\boldsymbol{S}_f}_{Diffusion-like} + \underbrace{\sum_{f\sim nb(C)} \dot{m}_f^*}_{Source-like} = 0$$

consists of a diffusion-like term $\sum_{f\sim nb(C)} -\rho_f \overline{\boldsymbol{D}_f^{\boldsymbol{v}}} (\nabla p'_f).\boldsymbol{S}_f$ of a gamma coefficient $\Gamma_f = -\rho_f \overline{\boldsymbol{D}_f^{\boldsymbol{v}}}$**.** It also includes a source term $\sum_{f\sim nb(C)} \dot{m}_f^*$.

The diffusion-like term is discretized into face fluxes such as:

$$fluxCf = -\Gamma_f^{\phi} gDiff_f = \rho_f \overline{\boldsymbol{D}_f^{\boldsymbol{v}}} gDiff_f$$

$$fluxFf = \Gamma_f^{\phi} gDiff_f = -\rho_f \overline{\boldsymbol{D}_f^{\boldsymbol{v}}} gDiff_f$$

$$fluxVf = -\rho_f \overline{\boldsymbol{D}_f^{\boldsymbol{v}}} \nabla p_f.\boldsymbol{T}_f$$

We introduce here $\mathcal{D}_f$:

$$\mathcal{D}_f = \overline{\boldsymbol{D}_f^{\boldsymbol{v}}} gDiff_f$$

So,

$$fluxCf = \rho_f \overline{\boldsymbol{D}_f^{\boldsymbol{v}}} gDiff_f = \rho_f \mathcal{D}_f$$

$$fluxFf = -\rho_f \overline{\boldsymbol{D}_f^{\boldsymbol{v}}} gDiff_f = -\rho_f \mathcal{D}_f$$

Usually, the non-linear flux of the diffusion term $-\rho_f \overline{\boldsymbol{D}_f^{\boldsymbol{v}}} \nabla p_f . \boldsymbol{T}_f$ is neglected, because it doesn't affect the final solution as it is a correction term, so the non-linear flux contribution of the diffusion-like term $fluxVf = 0$.

The source term $\sum_{f\sim NB} \dot{m}_f^*$ can be regarded as face fluxes contribution instead of element fluxes. So, the face flux contribution of the source term is:

$$fluxVf = \dot{m}_f^*$$

The total flux $fluxTf$ is:

$$fluxTf = fluxCfp_C + fluxFfp_F + fluxVf$$

Whereas for the compressible pressure correction equation

$$\underbrace{\frac{V_C C_\rho}{\Delta t} p'_C}_{Transient-like} + \underbrace{\sum_{f\sim nb(C)} C_{\rho,f} \left(\frac{\dot{m}_f^*}{\rho_f^*}\right) p'_f}_{Convection-like} + \underbrace{\sum_{f\sim nb(C)} -\rho_f \overline{\boldsymbol{D}_f^{\boldsymbol{v}}} (\nabla p'_f) . \boldsymbol{S}_f}_{Diffusion-like} + \underbrace{\frac{(\rho_C^* - \rho_C^\circ)}{\Delta t} + \sum_{f\sim nb(C)} \dot{m}_f^*}_{Source-like} = 0$$

there are additional terms (transient and convection). They are discretized regularly.

The transient term $\frac{V_C C_\rho}{\Delta t} p'_C$ element flux contribution is:

$$fluxC = \frac{V_C C_\rho}{\Delta t}$$

$$fluxC^\circ = 0$$

$$fluxV = 0$$

$$fluxT = fluxCp_C + fluxV$$

The convection term $\sum_{f\sim nb(C)} C_\rho \left(\frac{\dot{m}_f^*}{\rho_f^*}\right) p'_f$ has a psi coefficient $\psi_f = C_{\rho,f} \left(\frac{\dot{m}_f^*}{\rho_f^*}\right)$, so the face fluxes are:

$$fluxCf = \|\psi_f, 0\| = \left\| C_{\rho,f} \left(\frac{\dot{m}_f^*}{\rho_f^*}\right), 0 \right\|$$

$$fluxFf = -\|-\psi_f, 0\| = -\left\| -C_{\rho,f} \left(\frac{\dot{m}_f^*}{\rho_f^*}\right), 0 \right\|$$

$$fluxVf = 0$$

$$fluxTf = fluxCfp_C + fluxFfp_F + fluxVf$$

The source term includes an additional component. It is the $\frac{(\rho_C^* - \rho_C^\circ)}{\Delta t}$ term which is in fact a result of the transient term but will be here regarded as a source term because it is not standard.

$$fluxV = \frac{(\rho_C^* - \rho_C^\circ)}{\Delta t}$$

$$fluxT = fluxV$$

The corresponding code will be presented in the algebraic system section for convenience.

6.5.2.6 Pressure Correction Treatment for Free Surface Flow

In case the application is 'multiphase', uFVM is able to simulate homogeneous flows with a well-defined interface. In this case, the OpenFOAM case to be prepared is quite different, you may refer to the 'damBreak' case in the tutorials directory.

$$\sum_k \left\{ \frac{\partial(\alpha^k \rho^k)}{\partial t} + \nabla.(\alpha^k \rho^k \boldsymbol{v}) = \dot{M}^k \right\}$$

6.5.2.7 False Transience

For steady simulations, it is usually advantageous to insert a transient-like treatment. It acts as an under-relaxation to the equation yet is enhances diagonal dominance. It also adds a non-zero contribution to the diagonal coefficient even in the extreme cases where the diagonal coefficient is zero. Consider the following system:

$$a_C \phi_C + \sum_{F \sim NB(C)} a_F \phi_F = b_C$$

A false transient contributes to the equation above as shown here:

$$(a_C + a_C^\circ)\phi_C + \sum_{F \sim NB(C)} a_F \phi_F = b_C + a_C^\circ \phi_C^\circ$$

where

$$a_C^\circ = \frac{\rho_C V_C}{\Delta t}$$

The following listing is a retrieved from the function `cfdAssembleFalseTransientTerm` in the source files:

```
volumes = [theMesh.elements(iElements).volume]';
theFluxes.FLUXCE(iElements,1)    =   volumes .* rho / fdt;
theFluxes.FLUXCEOLD(iElements,1) = - volumes .* rho_old / fdt;
theFluxes.FLUXTE(iElements,1)    =   theFluxes.FLUXCE(iElements,1) .* phi;
theFluxes.FLUXTEOLD(iElements,1) =   theFluxes.FLUXCEOLD(iElements,1) .* phi_old;

cfdAssembleIntoGlobalMatrixElementFluxes(theEquationName,theFluxes,iComponent);
```

Listing 11 - Assembling false transience term

6.5.2.8 Gradient Computation

The gradient of a field ϕ can be calculated using Green-Gauss method. The gradient $\nabla\phi$ is calculated as follows:

$$\nabla\phi = \frac{1}{V_C}\sum_{f\sim nb(C)} \phi_f \boldsymbol{S}_f$$

However, the face value ϕ_f can be calculated in two approaches, a cell-based method and a node-base method. In the cell based method, the face value is calculated as the average values of the two cells sharing the face:

$$\phi_f = g_C\phi_C + (1-g_C)\phi_F$$

where g_C is the geometric weighing factor equal to

$$g_C = \frac{\|\boldsymbol{r}_F - \boldsymbol{r}_f\|}{\|\boldsymbol{r}_F - \boldsymbol{r}_C\|} = \frac{d_{Ff}}{d_{FC}}$$

The listing below shows the calculation of the face values and the gradient in the function `cfdComputeGradientGauss0`:

```
for iComponent=1:theNumberOfComponents
    phi_f = gf.*phi(iNeighbours,iComponent) + (1-gf).*phi(iOwners,iComponent);
    for iFace=iFaces
        phiGrad(iOwners(iFace),:,iComponent)     = phiGrad(iOwners(iFace),:,iComponent)     +
phi_f(iFace)*Sf(iFace,:);
        phiGrad(iNeighbours(iFace),:,iComponent) = phiGrad(iNeighbours(iFace),:,iComponent) -
phi_f(iFace)*Sf(iFace,:);
    end
end

%-----------------------------------------------------
% BOUNDARY FACES contribution to gradient
%-----------------------------------------------------
iBOwners = [theMesh.faces(iBFaces).iOwner]';
phi_b = phi(iBElements,:);
Sb = [theMesh.faces(iBFaces).Sf]';
for iComponent=1:theNumberOfComponents
    %
    for k=1:theMesh.numberOfBFaces
        phiGrad(iBOwners(k),:,iComponent) = phiGrad(iBOwners(k),:,iComponent) + phi_b(k)*Sb(k,:);
    end
end


%-----------------------------------------------------
% Get Average Gradient by dividing with element volume
%-----------------------------------------------------
volumes = [theMesh.elements(iElements).volume]';
for iComponent=1:theNumberOfComponents
    for iElement =1:theMesh.numberOfElements
        phiGrad(iElement,:,iComponent) = phiGrad(iElement,:,iComponent)/volumes(iElement);
    end
end
```

Listing 12 - Calculation of gradient based on Green-Gauss method

The node-based method requires that the node value is first calculated from the elements surrounding the node

$$\phi_n = \frac{\sum_{k=1}^{NB(n)} \frac{\phi_{F_k}}{\left\| \boldsymbol{r}_n - \boldsymbol{r}_{F_k} \right\|}}{\sum_{k=1}^{NB(n)} \frac{1}{\left\| \boldsymbol{r}_n - \boldsymbol{r}_{F_k} \right\|}}$$

And then the face value is calculated from the values of its nodes

$$\phi_f = \frac{\sum_{k=1}^{nb(f)} \frac{\phi_{n_k}}{\left\| \boldsymbol{r}_{n_k} - \boldsymbol{r}_f \right\|}}{\sum_{k=1}^{nb(f)} \frac{1}{\left\| \boldsymbol{r}_{n_k} - \boldsymbol{r}_f \right\|}}$$

The listing below in the function `cfdInterpolateFromElementsToNodes` calculates the values at the nodes:

```
for iNode = 1:numberOfNodes
    theNode = fvmNodes(iNode);
    N = theNode.centroid;

    localPhiNode=0;
    localInverseDistanceSum = 0;

    if(isempty(theNode.iFaces(theNode.iFaces>numberOfInteriorFaces)))
        localElementIndices = theNode.iElements;

        for iElement = localElementIndices
            theElement = fvmElements(iElement);
            C = theElement.centroid;

            d = cfdMagnitude(N-C);
            localPhi = phi(iElement);

            localPhiNode = localPhiNode + localPhi/d;
            localInverseDistanceSum = localInverseDistanceSum + 1/d;
        end
    else
        localBFacesIndices = theNode.iFaces(theNode.iFaces>numberOfInteriorFaces);
        for iBFace = localBFacesIndices
            theFace = fvmFaces(iBFace);
            C = theFace.centroid;
            iBElement = numberOfElements+(iBFace-numberOfInteriorFaces);

            d = cfdMagnitude(N-C);
            localPhi = phi(iBElement);

            localPhiNode = localPhiNode + localPhi/d;
            localInverseDistanceSum = localInverseDistanceSum + 1/d;
        end

    end
    localPhiNode = localPhiNode/localInverseDistanceSum;
    %
    %
    phi_n(iNode) = localPhiNode;
    %
end
```

Listing 13 - Interpolating the cell values to the nodes

Then the following code calculates the node values to the faces, and can be found in the function `cfdInterpolateFromNodesToFaces`:

```
for iFace=1:numberOfFaces

    theFace = fvmFaces(iFace);
    iNodes = theFace.iNodes;

    C = theFace.centroid;

    localSumOfInverseDistance=0;
    localPhi=0;
    for iNode=iNodes
        theNode = fvmNodes(iNode);
        N=theNode.centroid;
        d=cfdMagnitude(C-N);

        localPhi = localPhi + phiNodes(iNode)/d;
        localSumOfInverseDistance = localSumOfInverseDistance+1/d;
    end
    localPhi = localPhi/localSumOfInverseDistance;

    phi_f(iFace) = localPhi;
end
```

Listing 14 - Interpolating the node values to the faces

Finally, we calculate the gradient according to the Green-Gauss method which can be found in the function `cfdComputeGradientNodal`:

```
for iFace=1:theNumberOfInteriorFaces
   %
   theFace = fvmFaces(iFace);
   %
   iElement1 = theFace.iOwner;
   iElement2 = theFace.iNeighbour;
   %
   Sf = theFace.Sf;
   %
   %
   phiGrad(:,iElement1) = phiGrad(:,iElement1) + phi_f(iFace)*Sf;
   phiGrad(:,iElement2) = phiGrad(:,iElement2) - phi_f(iFace)*Sf;

end


%=====================================================
% BOUNDARY FACES contribution to gradient
%=====================================================
for iBPatch=1:theNumberOfBElements
    %
    iBFace = theNumberOfInteriorFaces+iBPatch;
    iBElement = theNumberOfElements+iBPatch;
    theFace = fvmFaces(iBFace);
    %
    iElement1 = theFace.iOwner;
    %
    Sb = theFace.Sf;
    phi_b = phi(iBElement);
    %
    phiGrad(:,iElement1) = phiGrad(:,iElement1) + phi_b*Sb;

end


%-----------------------------------------------------
% Get Average Gradient by dividing with element volume
%-----------------------------------------------------
for iElement =1:theNumberOfElements
   theElement = fvmElements(iElement);
   phiGrad(:,iElement) = phiGrad(:,iElement)/theElement.volume;
end
```

Listing 15 - Calculation of the Green-Gauss gradient based on the face values calculated from node values

6.5.2.9 Implicit Under-Relaxation

As suggested by Patankar's approach, a relaxation factor λ^{ϕ} is introduced into the algebraic system.

$$\frac{a_C}{\lambda^\phi}\phi_C + \sum_{F\sim NB(C)} a_F\phi_F = b_C + \frac{\left(1-\lambda^\phi\right)}{\lambda^\phi} a_C\phi_C^*$$

However, for an equation in the correction form, an implicit under-relaxation is made as follows:

$$\frac{a_C}{\lambda^\phi}\phi_C' + \sum_{F\sim NB(C)} a_F\phi_F' = b_C - \left(a_C\phi_C^* + \sum_{F\sim NB(C)} a_F\phi_F^*\right)$$

In uFVM, it is done in the function `cfdApplyURF`:

```
theEquation = cfdGetModel(theEquationName);

urf = theEquation.urf;

theCoefficients = cfdGetCoefficients;
theCoefficients.ac = theCoefficients.ac/urf;

cfdSetCoefficients(theCoefficients);
```

Listing 16 - Introducing under-relaxation to the algebraic equation

6.5.2.10 Residual Form of the Equation

In fact, uFVM assembles a residual or correction form of the equation instead of the direct equation. This correction makes use of the previous iteration values of ϕ_C such that:

$$\phi_C = \phi_C^* + \phi_C'$$

Satisfying in the standard equation form:

$$a_C(\phi_C^* + \phi_C') + \sum_{F\sim NB(C)} a_F(\phi_F^* + \phi_F') = b_C$$

$$\rightarrow\ a_C\phi_C' + \sum_{F\sim NB(C)} a_F\phi_F' = b_C - \left(a_C\phi_C^* + \sum_{F\sim NB(C)} a_F\phi_F^*\right)$$

Once the algebraic system is calculated and ϕ_C' is determined, the exact value ϕ_C is updated as:

$$\phi_C = \phi_C^* + \phi_C'$$

6.5.2.11 Residual Computation

The residuals are criteria upon which the user decides to consider the results correct enough. The residual R_C^ϕ of the algebraic equation at element C is calculated as:

$$R_C^\phi = \left| b_C - \left(a_C\phi_C + \sum_{F\sim NB(C)} a_F\phi_F\right)\right|$$

The maximum residual over the cells is calculated as:

$$R^{\phi}_{C,max} = \max\left(R^{\phi}_{C}\right)$$

And the root-mean-squared of the residuals over the cells is:

$$R^{\phi}_{C,rms} = \sqrt{\frac{\sum_{C\sim all\ cells}\left(R^{\phi}_{C}\right)^2}{number\ of\ elements}}$$

Normalized residuals provide better insight of the convergence. They are calculated as follows:

$$R^{\phi}_{C,scaled} = \frac{R^{\phi}_{C}}{\max(a_C\phi_C)}$$

After that, you we calculate the maximum and root-mean square scaled residual.

However, since in uFVM the equations are assembled in the residual (correction) form as mentioned earlier, the residual at element C is simply:

$$a_C\phi'_C + \sum_{F\sim NB(C)} a_F\phi'_F = b_C - \left(a_C\phi^*_C + \sum_{F\sim NB(C)} a_F\phi^*_F\right) =$$

So,

$$R^{\phi}_{C} = \left|b_{C,res}\right|$$

The following listing presents the residual calculation; it is available in the function `cfdComputeNormalizedResidual`:

```
% Loop over elements and calculate residual at each element
Rc = abs(bc);

% Residuals. Calculate for convenience. Otherwise, they are not used
Rc_max = max(Rc);
Rc_rms = sqrt(sum(Rc.^2)/theNumberOfElements);

% Get phi scale from data base.
% phi_scale = max(abs(phi)). And if phi is zero, phi_scale is set to 1
phi_scale = cfdGetScale(theEquationUserName);

% Normalized Residuals
Rc_scaled = Rc / (max(abs(ac))*phi_scale);
Rc_max_scaled = max(Rc_scaled);
Rc_rms_scaled = sqrt(sum(Rc_scaled.^2)/theNumberOfElements);

MAXResidual = Rc_max_scaled;
RMSResidual = Rc_rms_scaled;
```

Listing 17 - Residual calculation

A special case arises with the pressure correction equation as it is by default in the correction form as shown here:

$$a_C p'_C + \sum_{F \sim NB(C)} a_F p'_F = b_C^p$$

However, the residual of this equation is determined as a continuity criterion

$$\nabla . \boldsymbol{v} = 0$$

$$\rightarrow \sum_{f \sim nb(C)} \dot{m}_f = 0$$

Thus, a quantity called $Div_{effective} = \sum_{f \sim nb(C)} \dot{m}_f$ is calculated at each iteration to judge the convergence of the continuity equation, so, we have for the continuity equation:

$$R_C^{\phi} = Div_{effective}$$

The corresponding implementation can be found in the function: `cfdComputeEffectiveDivergence`:

```
% Interior Faces Contribution
theNumberOfInteriorFaces = cfdGetNumberOfInteriorFaces;
iFaces = 1:theNumberOfInteriorFaces;
owners = [theMesh.faces(iFaces).iOwner]';
neighbours = [theMesh.faces(iFaces).iNeighbour]';
for iFace=1:theNumberOfInteriorFaces
    iOwner = owners(iFace);
    iNeighbour = neighbours(iFace);
    %
    effDiv(iOwner)     = effDiv(iOwner)     + mdot_f(iFace);
    effDiv(iNeighbour) = effDiv(iNeighbour) - mdot_f(iFace);
end

% Boundary Faces Contribution
theNumberOfPatches = cfdGetNumberOfPatches;
for iPatch=1:theNumberOfPatches
    theBoundary = theMesh.boundaries(iPatch);
    numberOfBFaces = theBoundary.numberOfBFaces;

    % cfdGetBoundaryIndex
    iFaceStart = theBoundary.startFace;
    iFaceEnd = iFaceStart+numberOfBFaces-1;
    iBFaces = iFaceStart:iFaceEnd;

    owners = [theMesh.faces(iBFaces).iOwner]';
    mdot_b = theMdotField.phi(iBFaces);

    for iBFace=1:numberOfBFaces
        iOwner = owners(iBFace);
        effDiv(iOwner) = effDiv(iOwner) + mdot_b(iBFace);
    end
end
```

Listing 18 - Calculating the effective divergence as a residual criterion for the continuity equation

6.5.2.12 Assembling Fluxes to Global Assembly Matrix

After calculating the face or/and element fluxes from each term, these fluxes are to be summed to construct the algebraic system coefficients.

6.5.2.12.1 Algebraic Systems Representation

The algebraic system $A\phi' = b$ is constructed:

$$\begin{bmatrix} a_{11} & \dots & a_{1N} \\ \vdots & \ddots & \vdots \\ a_{N1} & \dots & a_{NN} \end{bmatrix} \begin{bmatrix} \phi'_1 \\ \vdots \\ \phi'_N \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_N \end{bmatrix}$$

The coefficient matrix A is a highly sparse matrix, so it is stored as an array for the diagonal coefficients in addition of a data structure containing the non-zeros at each row (off-diagonal coefficients). The diagonal array is named in uFVM as `ac` and the off-diagonal coefficient data structure as `anb`.

6.5.2.12.2 Assembling Algebraic System coefficients

If the discretized term gives rise to element fluxes like the transient and source terms, the fluxes $fluxC$, $fluxC^{\circ}$, $fluxV$ and $fluxT$ are assembled as follows given that the algebraic equation is in the residual (correction) form:

$$a_C = a_C + fluxC$$

$$a_C^{\circ} = a_C^{\circ} + fluxC^{\circ}$$

$$b_C = b_C - fluxT$$

If the term includes faces fluxes ($fluxCf$, $fluxFf$, $fluxVf$ and $fluxTf$) like the convection and diffusion terms, the assembling is done such as:

$$a_C = a_C + \sum_{f \sim nb(C)} fluxCf$$

$$a_F = a_F + fluxFf$$

$$b_C = b_C - \sum_{f \sim nb(C)} fluxTf$$

Recall that for element fluxes:

$$fluxT = fluxC\phi_C^* + fluxC^{\circ}\phi_C^{\circ} + fluxV$$

And for face fluxes,

$$fluxTf = fluxCf\phi_C^* + fluxFf\phi_F^* + fluxVf$$

Therefore, the algebraic equation has the general form:

$$\underbrace{\left(fluxC + \sum_{f \sim nb(C)} FluxCf\right)}_{a_C}\phi_C' + \sum_{\substack{F \sim NB(C) \\ f \sim nb(C)}} \underbrace{FluxCf}_{a_F}\phi_F' = \underbrace{-\left(fluxT + \sum_{f \sim nb(C)} FluxTf\right)}_{b_C}$$

So,

$$a_C = fluxC + \sum_{f \sim nb(C)} FluxCf$$

$$a_F = FluxCf$$

$$b_C = -\left(fluxT + \sum_{f\sim nb(C)} FluxTf \right)$$

The pressure equation again has a special case since it is already in the residual form. The discretized incompressible pressure correction equation:

$$\underbrace{\left(\sum_{f\sim nb(C)} \rho_f \mathcal{D}_f \right)}_{a_C} p'_C + \sum_{\substack{F\sim NB(C) \\ f\sim nb(C)}} \underbrace{-\rho_f \mathcal{D}_f}_{a_F} p'_F = \underbrace{-\sum_{f\sim nb(C)} \dot{m}^*_f}_{b_C}$$

So, the fluxes here are to be calculated as:

1) Diagonal coefficient a_C:

$$a_C = fluxC + \sum_{f\sim nb(C)} FluxCf = \sum_{f\sim nb(C)} \rho_f \mathcal{D}_f$$

$$\rightarrow fluxC = 0 \text{ and } FluxCf = \rho_f \mathcal{D}_f$$

2) Off-diagonal coefficients a_F:

$$a_F = FluxFf = -\rho_f \mathcal{D}_f$$

3) Right-hand-side:

$$b_C = -\left(fluxT + \sum_{f\sim nb(C)} FluxTf \right) = -\sum_{f\sim nb(C)} \dot{m}^*_f$$

$$\rightarrow fluxT = 0 \text{ and } FluxTf = \dot{m}^*_f$$

For the compressible pressure correction equation, the discretized equation is:

$$\underbrace{\left(\frac{V_C C_\rho}{\Delta t} + \sum_{f\sim nb(C)} \left(\frac{C_{\rho,f}}{\rho^*_f} \left\| \dot{m}^*_f, 0 \right\| \right) + \sum_{f\sim nb(C)} \rho^*_f \mathcal{D}_f \right)}_{a_C} p'_C + \sum_{\substack{F\sim NB(C) \\ f\sim nb(C)}} \underbrace{\left(-\frac{C_{\rho,f}}{\rho^*_f} \left\| -\dot{m}^*_f, 0 \right\| - \rho^*_f \mathcal{D}_f \right)}_{a_F} p'_F = \underbrace{-\sum_{f\sim nb(C)} \dot{m}^*_f - \frac{(\rho^*_C - \rho^\circ_C)}{\Delta t}}_{b_C}$$

So, the fluxes of the compressible pressure correction equation are calculated as:

1) Diagonal coefficient a_C:

$$a_C = fluxC + \sum_{f\sim nb(C)} FluxCf = \frac{V_C C_\rho}{\Delta t} + \sum_{f\sim nb(C)} \left(\frac{C_{\rho,f}}{\rho_f^*} \left\| \dot{m}_f^*, 0 \right\| \right) + \sum_{f\sim nb(C)} \rho_f^* \mathcal{D}_f$$

$$\rightarrow fluxC = \frac{V_C C_\rho}{\Delta t} \text{ and } FluxCf = \frac{C_{\rho,f}}{\rho_f^*} \left\| \dot{m}_f^*, 0 \right\| + \rho_f^* \mathcal{D}_f$$

2) Off-diagonal coefficients a_F:

$$a_F = FluxFf = -\frac{C_{\rho,f}}{\rho_f^*} \| -\dot{m}_f^*, 0 \| - \rho_f^* \mathcal{D}_f$$

3) Right-hand-side:

$$b_C = -\left(fluxT + \sum_{f\sim nb(C)} FluxTf \right) = -\left(\frac{(\rho_C^* - \rho_C^\circ)}{\Delta t} + \sum_{f\sim nb(C)} \dot{m}_f^* \right)$$

$$\rightarrow fluxT = \frac{(\rho_C^* - \rho_C^\circ)}{\Delta t} \text{ and } FluxTf = \dot{m}_f^*$$

The listing below shows the calculation of the fluxes of the pressure correction equation:

```
%
% assemble term I
%     rho_f [v]_f.Sf
%
U_bar_f = dot(vel_bar_f(:,:)',Sf(:,:)')';
FLUXVf = FLUXVf + rho_f.*U_bar_f;
%
% Assemble term II and linearize it
%      - rho_f ([DPVOL]_f.P_grad_f).Sf
%
DUSf = [DU1_f.*Sf(:,1),DU2_f.*Sf(:,2),DU3_f.*Sf(:,3)]; % S'f
eDUSf = [DUSf(:,1)./cfdMagnitude(DUSf),DUSf(:,2)./cfdMagnitude(DUSf),DUSf(:,3)./cfdMagnitude(DUSf)];

DUEf =
[cfdMagnitude(DUSf).*eCN(:,1)./dot(eCN(:,:)',eDUSf(:,:)')',cfdMagnitude(DUSf).*eCN(:,2)./dot(eCN(:,:)',eDUSf(:,:)'
)',cfdMagnitude(DUSf).*eCN(:,3)./dot(eCN(:,:)',eDUSf(:,:)')'];
geoDiff = cfdMagnitude(DUEf)./cfdMagnitude(CN);

DUTf = DUSf - DUEf;

FLUXCf = FLUXCf + rho_f.*geoDiff;
FLUXFf = FLUXFf - rho_f.*geoDiff;
FLUXVf  = FLUXVf  - rho_f.*dot(p_grad_f(iFaces,:)',DUTf(:,:)')';
%
%  assemble term III
%    rho_f ([P_grad]_f.([DPVOL]_f.Sf))
%
FLUXVf = FLUXVf + rho_f.*dot(p_grad_bar_f(iFaces,:)',DUSf(:,:)')';
%
% assemble terms VIII and IX
%     (1-URF)(U_f -[v]_f.S_f)
%
FLUXVf = FLUXVf + (1.0 - mdot_f_URF)*(mdot_f_previous - rho_f.*U_bar_f);
%
% compute Rhie-Chow interpolation of mdot_f and updated it in the data base
%
mdot_f = FLUXCf .* pressureC + FLUXFf .* pressureN + FLUXVf;
theMdotField.phi(iFaces) = mdot_f;
cfdSetMeshField(theMdotField);
%
% assemble total flux
%
FLUXTf = mdot_f;
%
% assemble terms X (for compressible flow)
%
applicationClass = cfdGetApplicationClass;
if strcmp(applicationClass, 'compressible')
    theDrhodpField = cfdGetMeshField('C_rho');
    C_rho = theDrhodpField.phi;
    C_rho_f = cfdInterpolateFromElementsToFaces('Average', C_rho);
    C_rho_f = C_rho_f(iFaces);

    FLUXCf = FLUXCf + (C_rho_f ./ rho_f) .* max(mdot_f, 0);
    FLUXFf = FLUXFf - (C_rho_f ./ rho_f) .* max(-mdot_f, 0);

    % Add transient contribution
    if isTransient
        deltaT = cfdGetDt;
        volume = [theMesh.elements.volume]';

        FLUXCE = volume(iElements) .* C_rho(iElements) / deltaT;
        FLUXTE = (rho(iElements) - density_old(iElements)) .* volume(iElements) / deltaT ;
    end
end
```

Listing 19 - Calculating fluxes of the pressure correction equation

In uFVM, the assembling of element fluxes is shown here in the listing below retrieved from the function `cfdAssembleIntoGlobalMatrixElementFluxes`:

```
% Call coefficients
ac = theCoefficients.ac;
ac_old = theCoefficients.ac_old;
bc = theCoefficients.bc;

% Assemble element fluxes
for iElement = 1:numberOfElements
    ac(iElement)     = ac(iElement)     + theFluxes.FLUXCE(iElement);
    ac_old(iElement) = ac_old(iElement) + theFluxes.FLUXCEOLD(iElement);
    bc(iElement)     = bc(iElement)     - theFluxes.FLUXTE(iElement);
end

% Store updated coefficients
theCoefficients.ac = ac;
theCoefficients.ac_old = ac_old;
theCoefficients.bc = bc;
```

Listing 20 - Assembling element fluxes

The assembly of face fluxes is shown here, and it is retrieved from the function `cfdAssembleIntoGlobalMatrixFaceFluxes`:

```
% Call coefficients
ac = theCoefficients.ac;
anb = theCoefficients.anb;
bc = theCoefficients.bc;
%
% Assemble fluxes of interior faces
%
for iFace = 1:numberOfInteriorFaces
    theFace                 = theMesh.faces(iFace);
    iOwner                  = theFace.iOwner;
    iOwnerNeighbourCoef     = theFace.iOwnerNeighbourCoef;
    iNeighbour              = theFace.iNeighbour;
    iNeighbourOwnerCoef     = theFace.iNeighbourOwnerCoef;
    %
    %  assemble fluxes for owner cell
    %
    ac(iOwner)                      = ac(iOwner)                      + theFluxes.FLUXC1f(iFace);
    anb{iOwner}(iOwnerNeighbourCoef) = anb{iOwner}(iOwnerNeighbourCoef) + theFluxes.FLUXC2f(iFace);
    bc(iOwner)                      = bc(iOwner)                      - theFluxes.FLUXTf(iFace);
    %
    %  assemble fluxes for neighbour cell
    %
    ac(iNeighbour)                      = ac(iNeighbour)                      - theFluxes.FLUXC2f(iFace);
    anb{iNeighbour}(iNeighbourOwnerCoef) = anb{iNeighbour}(iNeighbourOwnerCoef) - theFluxes.FLUXC1f(iFace);
    bc(iNeighbour)                      = bc(iNeighbour)                      + theFluxes.FLUXTf(iFace);
end
%
% assemble fluxes of boundary faces
%
for iBFace=numberOfInteriorFaces+1:numberOfFaces
    theBFace = theMesh.faces(iBFace);
    iOwner         = theBFace.iOwner;
    %
    %  assemble fluxes for owner cell
    %
    ac(iOwner) = ac(iOwner) + theFluxes.FLUXC1f(iBFace);
    bc(iOwner) = bc(iOwner) - theFluxes.FLUXTf(iBFace);
end

% Store updated coefficients
theCoefficients.ac = ac;
theCoefficients.anb = anb;
theCoefficients.bc = bc;
```

Listing 21 - Assembling face fluxes

6.5.3 Solving the Equation Algebraic System

The algebraic system is solved $A\phi' = b$ iteratively. Direct solving of the system using Gaussian elimination is very expensive because the matrix A is usually large and highly sparse. There are plenty of solvers which iteratively try to approximate the solution of the system. In uFVM, two iterative solvers are implemented, Successive Over-relaxation (SOR) and Incomplete Lower Upper (ILU).

6.5.3.1 SOR Solver

The SOR is a Gauss-Seidal solver except that it includes a factor ω which enhances the progress of the solver. Check the function `cfdSORSolver`:

```
for iElement=1:numberOfElements
    cconn = theCoefficients.cconn{iElement};
    local_dphi = bc(iElement);
    for iLocalNeighbour = 1:length(cconn)
        iNeighbour = cconn(iLocalNeighbour);
        local_dphi = local_dphi - anb{iElement}(iLocalNeighbour)*dphi(iNeighbour);
    end
    dphi(iElement) = local_dphi/ac(iElement);
end

for iElement=numberOfElements:-1:1
    cconn = theCoefficients.cconn{iElement};
    local_dphi = bc(iElement);
    for iLocalNeighbour = 1:length(cconn)
        iNeighbour = cconn(iLocalNeighbour);
        local_dphi = local_dphi - anb{iElement}(iLocalNeighbour)*dphi(iNeighbour);
    end
    dphi(iElement) = local_dphi/ac(iElement);
end
```

Listing 22 - SOR solver

6.5.3.2 ILU Solver

Incomplete factorization of the matrix A is an efficient preconditioner which allows for an accelerated convergence rate of the solver. The corresponding function is: `cfdILUSolver`

```
for i1=1:numberOfElements
    dc(i1) = ac(i1);
end

for i1=1:numberOfElements
    dc(i1) = 1.0/dc(i1);
    rc(i1) = bc(i1);

    i1NbList = theCoefficients.cconn{i1};
    i1NNb = length(i1NbList);

    if(i1~=numberOfElements-1)
        % loop over neighbours of iElement
        j1_ = 1;
        while(j1_<=i1NNb)
            jj1 = i1NbList(j1_);
            % for all neighbour j > i do
            if((jj1>i1) && (jj1<=numberOfElements))
                j1NbList = theCoefficients.cconn{jj1};
                j1NNb = length(j1NbList);
                i1_= 0;
                k1 = -1;
                % find _i index to get A[j][_i]
                while((i1_<=j1NNb) && (k1 ~= i1))
                    i1_ = i1_ + 1;
                    k1 = j1NbList(i1_);
                end
                % Compute A[j][i]*D[i]*A[i][j]
                if(k1 == i1)
                    dc(jj1) = dc(jj1) - anb{jj1}(i1_)*dc(i1)*anb{i1}(j1_);
                else
                    disp('the index for i in j is not found');
                end
            end
            j1_ = j1_ + 1;
        end
    end
end
```

Listing 23 - ILU solver

6.5.3.3 AMG Linear Solver

An algebraic multigrid solver remove low-frequency error components. In the context of multigrid solvers, the direct iterative solvers like *ILU* solver are regarded as smoothers. Below is

a glance to the AMG code, it is advisable to access the code to see much more details about it. Refer to `cfdApplyAMG`.

```
gridLevel = 1;
nCycle = 1;
if(strcmp(cycleType,'V-Cycle'))
    while ((nCycle<=maxCycles)&&(finalResidual>rrf*initialResidual))
        %
        % Apply V-Cycle
        %
        finalResidual = cfdApplyVCycle(gridLevel,smootherType,maxLevels,preSweep,postSweep,rrf);
        %
        nCycle = nCycle + 1;
    end
elseif(strcmp(cycleType,'F-Cycle'))
    while ((nCycle<=maxCycles)&&(finalResidual>rrf*initialResidual))
        %
        % Apply F-Cycle
        %
        finalResidual = cfdApplyFCycle(gridLevel,smootherType,maxLevels,preSweep,postSweep,rrf);
        %
        nCycle = nCycle + 1;
    end
elseif(strcmp(cycleType,'W-Cycle'))
    while ((nCycle<=maxCycles)&&(finalResidual>rrf*initialResidual))
        %
        % Apply W-Cycle
        %
        finalResidual = cfdApplyWCycle(gridLevel,smootherType,maxLevels,preSweep,postSweep,rrf);
        %
        nCycle = nCycle + 1;
    end
end
```

Listing 24 - Multigrid solver

Note: uFVM utilizes the AMG solver by default for the pressure equation only, while applies direct iterative solvers for all other equations.

6.5.4 Correcting Equation Solution

All the equations are corrected just after solving the algebraic system $A\phi' = b$ such that:

$$\phi_C = \phi_C^* + \phi_C'$$

However, after solving the pressure correction equation, the other fields have also to be corrected:

For incompressible flow:

$$\boldsymbol{v}_C^{**} = \boldsymbol{v}_C^* - \boldsymbol{D}_C^{\boldsymbol{v}}(\nabla p')_C$$

$$p_C^* = p_C^{(n)} + \lambda^p p_C'$$

$$\dot{m}_f^{**} = \dot{m}_f^* - \rho_f^* \overline{\boldsymbol{D}_f^{\boldsymbol{v}}} \nabla p_f' . \boldsymbol{S}_f$$

For compressible flow:

$$\boldsymbol{v}_C^{**} = \boldsymbol{v}_C^* - \boldsymbol{D}_C^{\boldsymbol{v}}(\nabla p')_C$$

$$p_C^* = p_C^{(n)} + \lambda^p p_C'$$

$$\rho_C^{**} = \rho_C^* + \lambda^\rho C_\rho p_C'$$

$$\dot{m}_f^{**} = \dot{m}_f^* - \rho_f^* \overline{\boldsymbol{D}_f^{\boldsymbol{v}}} \nabla p_f' . \boldsymbol{S}_f + \left(\frac{\dot{m}_f^*}{\rho_f^*} \right) C_{\rho,f} p_f'$$

Listing of correcting $\dot{m}_f^*$:

```
applicationClass = cfdGetApplicationClass;
if strcmp(applicationClass, 'compressible')
    % Get density field
    theDensityField = cfdGetMeshField('rho');
    rho = theDensityField.phi;

    % Get the convected density at the faces
    pos = zeros(size(mdot_f));
    pos(mdot_f>0) = 1;
    rho_f = rho(iOwners).*pos(iFaces) + rho(iNeighbours).*(1 - pos(iFaces));

    % Get drhodp field
    theDrhodpField = cfdGetMeshField('C_rho');
    C_rho = theDrhodpField.phi;
    C_rho_f = cfdInterpolateFromElementsToFaces('Average', C_rho);
    C_rho_f = C_rho_f(iFaces);

    % Correct bt adding compressible contribution
    mdot_f(iFaces) = mdot_f(iFaces) + (mdot_f(iFaces) ./ rho_f) .* C_rho_f .* pp(iOwners);
end

% Correct
mdot_f(iFaces) = mdot_f(iFaces) + FLUXC1f(iFaces).*pp(iOwners) + FLUXC2f(iFaces).*pp(iNeighbours);
```

Listing 25 - Correcting $\dot{m}_f^*$

Listing of correcting $\boldsymbol{v}_C^*$:

```
thePPField = cfdGetMeshField('PP');
ppGrad = thePPField.phiGradient;
%
DUPPGRAD = [DU1.*ppGrad(iElements,1),DU2.*ppGrad(iElements,2),DU3.*ppGrad(iElements,3)];
%
theVelocityField = cfdGetMeshField('U');
vel = theVelocityField.phi;
%
vel(iElements,:) = vel(iElements,:) - DUPPGRAD(iElements,:);
```

Listing 26 – Correcting $\boldsymbol{v}_C^*$

Listing of correcting ρ_C^*:

```
thePressureCorrectionField = cfdGetMeshField('PP');
pp = thePressureCorrectionField.phi;

theDensityField = cfdGetMeshField('rho');
rho = theDensityField.phi;

theDrhodpField = cfdGetMeshField('C_rho');
C_rho = theDrhodpField.phi;

theEquation = cfdGetModel('rho');
URFRho = theEquation.urf;

rho = rho + 0.7 .* C_rho .* pp;
```

Listing 27 – Correcting ρ_C^*

Further details of the implementation of field corrections can be found at `cfdCorrectEquation`.

6.6 CONVERGENCE

Once the case is run, the solution will be updated at each iteration while at the mean time a real-time plot will be displayed showing the residuals of the equations. A sample is shown in the figure below:

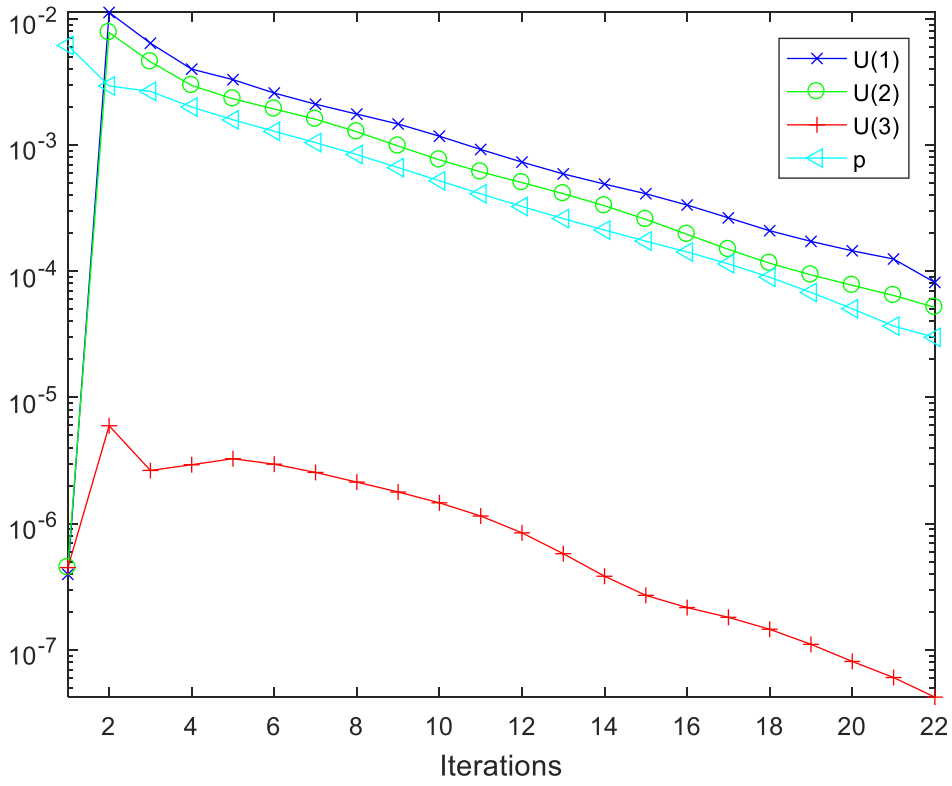


Figure 4 - Real-time residuals monitor

Once the case is run until convergence, or the maximum number of iterations are reached in a steady state simulation, a phrase '*Solution is converged!*' will show up on the screen notifying the user.

In case of divergence, a pop-up message box will be displayed notifying the user that the program has detected divergence. The box is presented below:

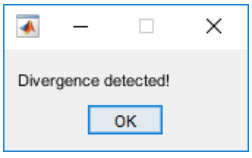


Figure 5 - Divergence notification

6.7 POST-PROCESSING

The user may plot the results on figures. The corresponding functions to plot the resulting fields is `cfdPlotField`. The function takes an argument the name of the field to be plotted. Considering that the user wants to plot the velocity field, they have to call the following in the command window:

```
cfdPlotField('U')
```

To plot the velocity vectors, the function to be used is `cfdPlotVelocity`. The function takes as arguments the vector scale, the transparency of the faces and the vector skipping criterion. If the user wants to plot the vector field with vector scale of 1, full transparency and 10 vector skips (skip a vector every 10 vectors), they have to call the following in the command window:

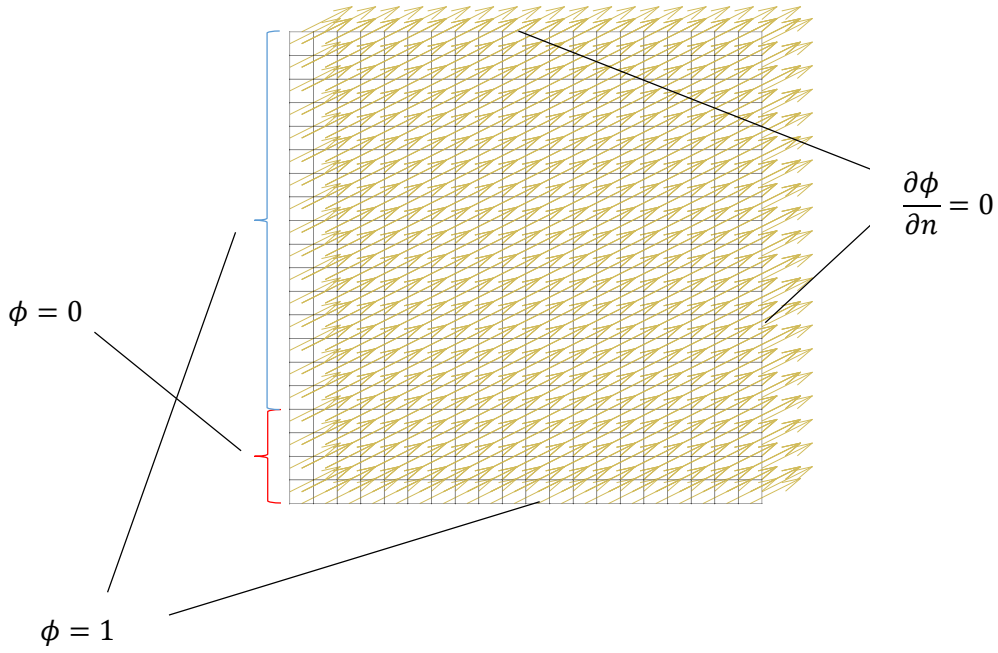
```
cfdPlotVelocity('vectorScale',1,'faceAlpha',0,'vectorSkip',0);
```

7 TUTORIALS

In this chapter, some tutorials will be provided from each application class. 5 application classes can be simulated so far within uFVM: basic, incompressible, compressible, Heat Transfer and multiphase.

7.1 BASIC

The 'stepProfile' case is considered here. The mesh is a square domain with 20 by 20 structured cells. A constant velocity profile ($2\hat{\imath} + 1\hat{\jmath}$) is assumed over the domain as shown in the figure below. We attempt to solve a pure convection problem in order to evaluate the quality of convection schemes. The convected quantity is ϕ and has dirichlet boundary conditions at two patches shown below in the figure, while on the other part of the boundary, the quantity ϕ is set to zero gradient.



The equation that is to be solved is

$$\nabla.(\rho \boldsymbol{v} \phi) = 0$$

where $\boldsymbol{v}$ is the velocity field set as constant field (Refer to the 0 directory in the tutorials and look at the file named 'U'). The corresponding run file is as shown here:

```
%--------------------------------------------------------------------------
%
%  written by the CFD Group @ AUB, 2017
%  contact us at: cfd@aub.edu.lb
%==========================================================================
% Case Description:
%     In this test case the square cavity problem is considered with a
%     uniform velocity profile throughout the domain. The objective is to
%     investigate the convection schemes (the default now is set to first
%     order upwind).
%--------------------------------------------------------------------------

% Setup Case
cfdSetupSolverClass('basic');

% Read OpenFOAM Files
cfdReadOpenFoamFiles;

% Setup Time Settings
cfdSetupTime;

% Setup Equations
cfdDefineEquation('phi', 'div(rho*U*phi) = 0'); % Convection

% Initialize case
cfdInitializeCase;

% Run case
cfdRunCase;
```

In addition, we set the default option of the divSchemes in the 'fvShemes' directory to 'Gauss upwind' which corresponds to first order upwind. Running the case generates the following residuals plot:

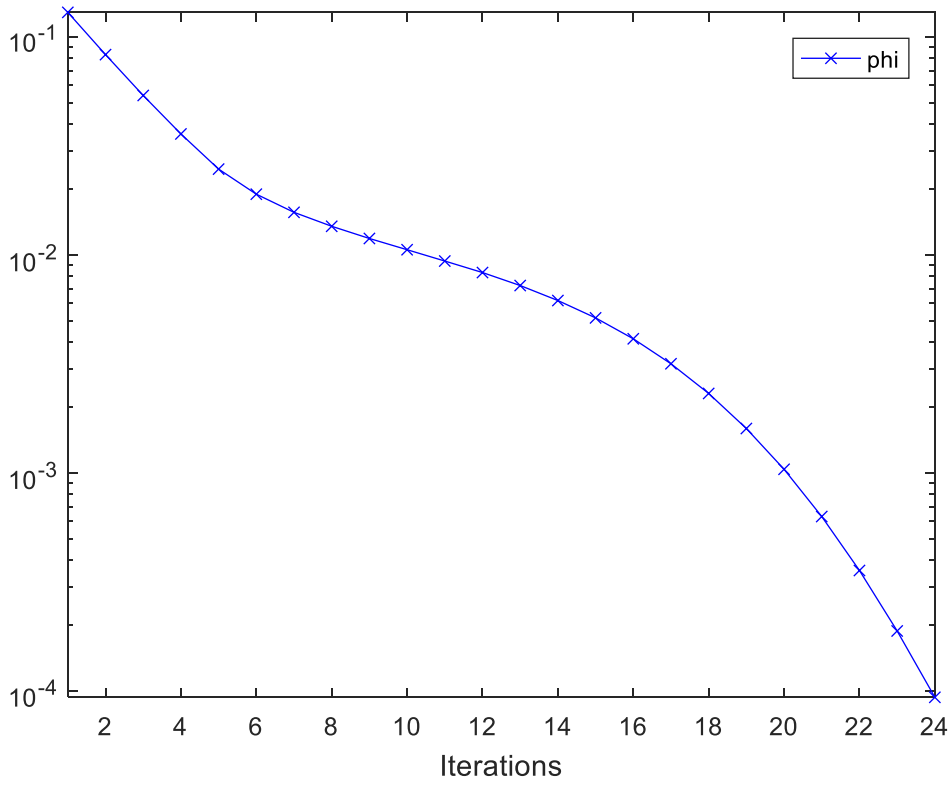


Figure 6 - Residuals monitor for the upwind convection of the quantity ϕ

The contour of ϕ is as follows:

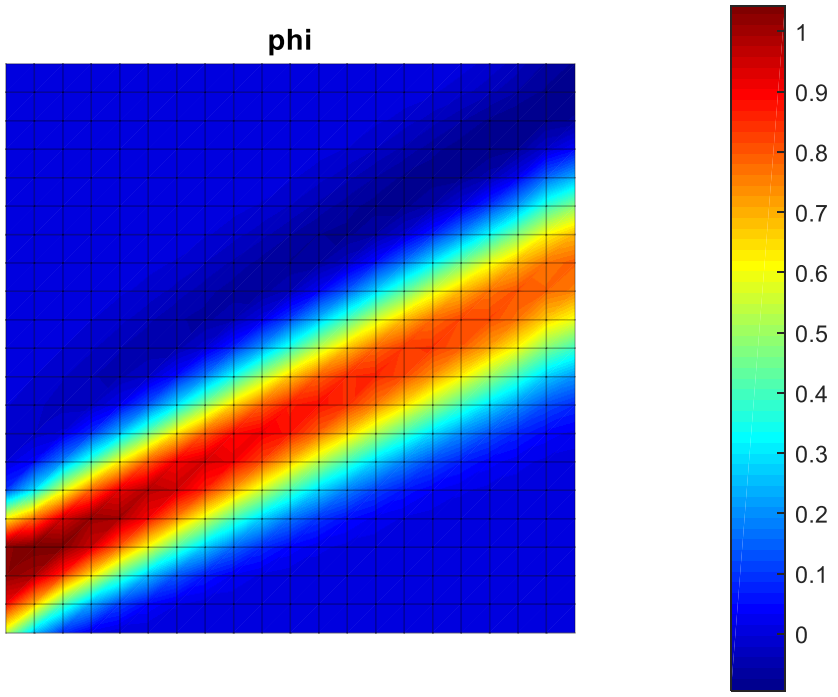
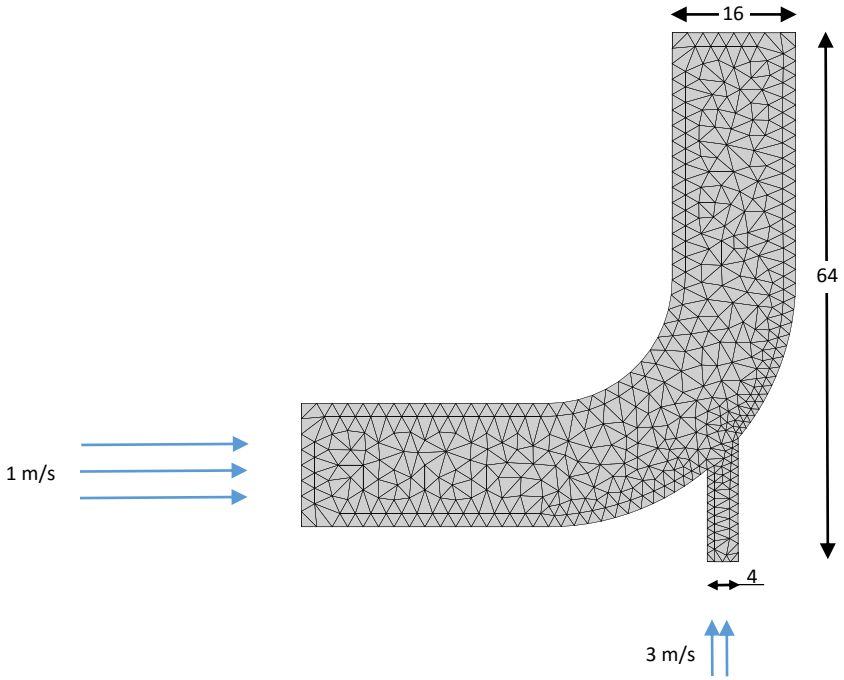


Figure 7 - Contour plot of phi subject to first order upwind convection

7.2 INCOMPRESSIBLE

The 'elbow' case is considered here. The following is the mesh with inlet velocities shown:



This case simulates a water flow in the elbow at steady state conditions with no gravitational acceleration. The governing equations are:

Momentum:

$$\nabla.(\rho \boldsymbol{v}\boldsymbol{v}) = \mu\nabla^2\boldsymbol{v} + \nabla.\{\mu(\nabla\boldsymbol{v})^T\} - \nabla p$$

Continuity:

$$\nabla.\boldsymbol{v} = 0$$

Energy:

$$\nabla.\left(\rho c_p \boldsymbol{v} T\right) = k\nabla^2 T$$

The corresponding run case is:

```
%--------------------------------------------------------------------------
%
%  written by the CFD Group @ AUB, 2017
%  contact us at: cfd@aub.edu.lb
%==========================================================================
% Case Description:
%     In this test case a water flow in an elbow is simulated at steady state
%--------------------------------------------------------------------------

% Setup Case
cfdSetupSolverClass('incompressible');

% Read OpenFOAM Files
cfdReadOpenFoamFiles;

% Setup Time Settings
cfdSetupTime;

% Setup Equations
cfdDefineEquation('U', 'div(rho*U*U) = laplacian(mu*U) + div(mu*transp(grad(U))) - grad(p)'); % Momentum
cfdDefineEquation('p', 'div(U) = 0'); % Continuity
cfdDefineEquation('T', 'div(rho*Cp*U*T) = laplacian(k*T)'); % Energy

% Initialize case
cfdInitializeCase;

% Run case
cfdRunCase;
```

Listing 28 - Run file of the 'elbow' case

Refer to the ‘elbow’ case in the tutorials directory. Running the case will solve the problem where it converges after 105 iterations, and the figure below shows the residuals history of the equations (U, p, and T):

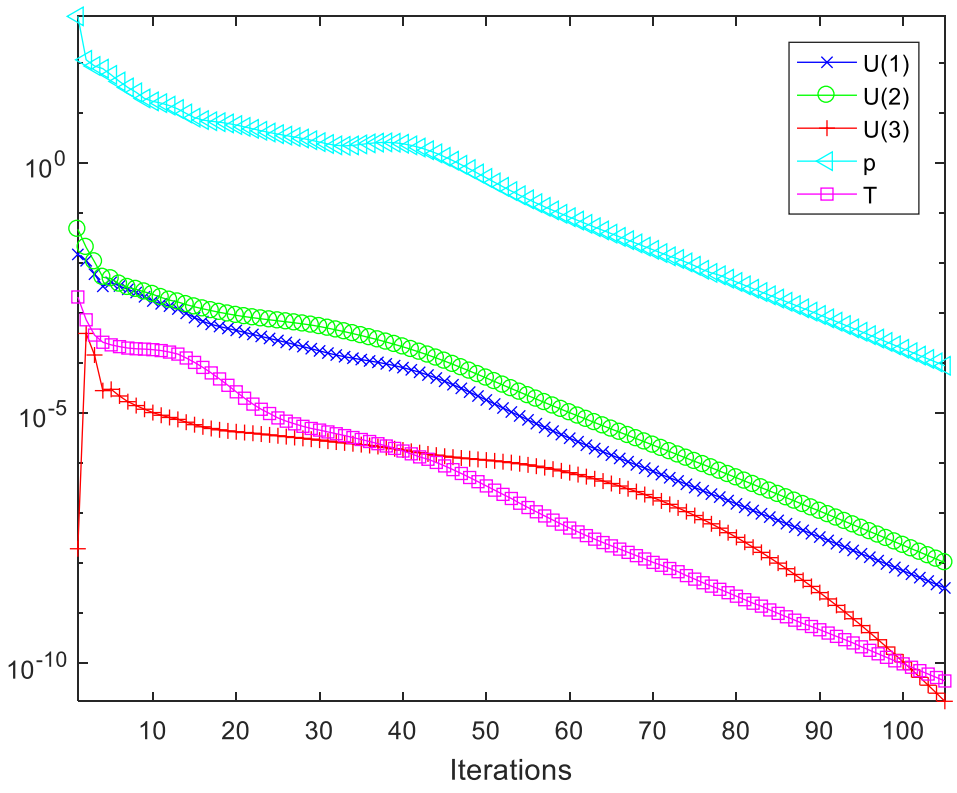


Figure 8 - Residuals history of the elbow case

We call the following functions:

```
cfdPlotField('U')
cfdPlotField('p')
cfdPlotField('T')
cfdPlotVelocity('vectorScale',1,'faceAlpha',0,'vectorSkip',0);
```

The results for velocity ‘U’, pressure ‘p’ and temperature ‘T’ in addition to the velocity vector field will be plotted. Presented below are the results:

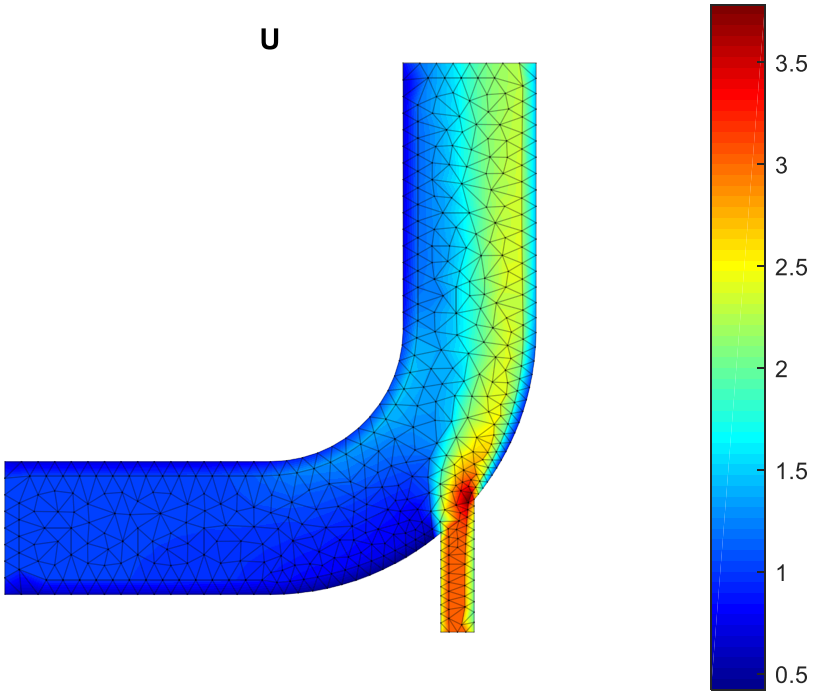


Figure 9 - Velocity magnitude contour (m/s)

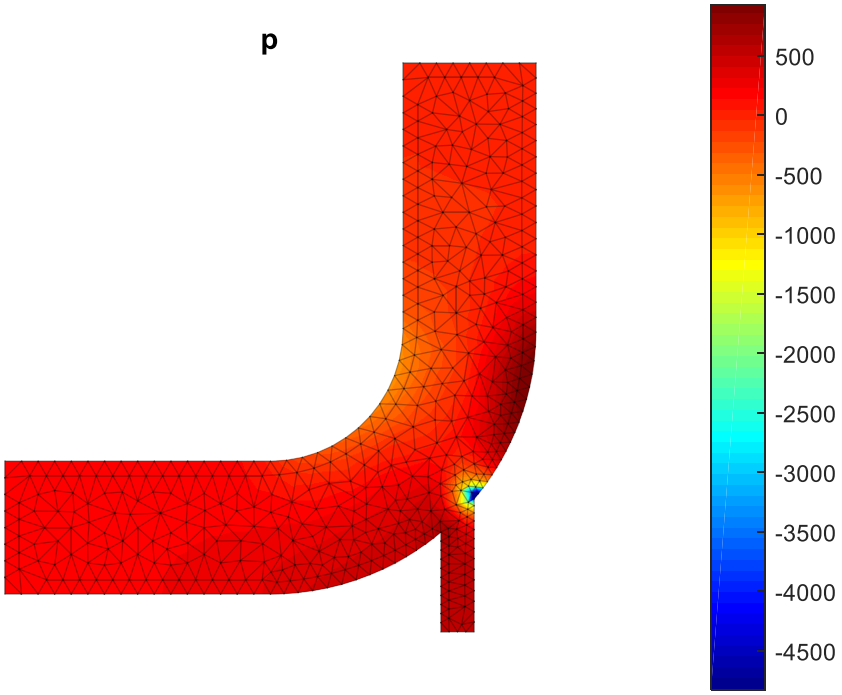


Figure 10 - Pressure contour (pa)

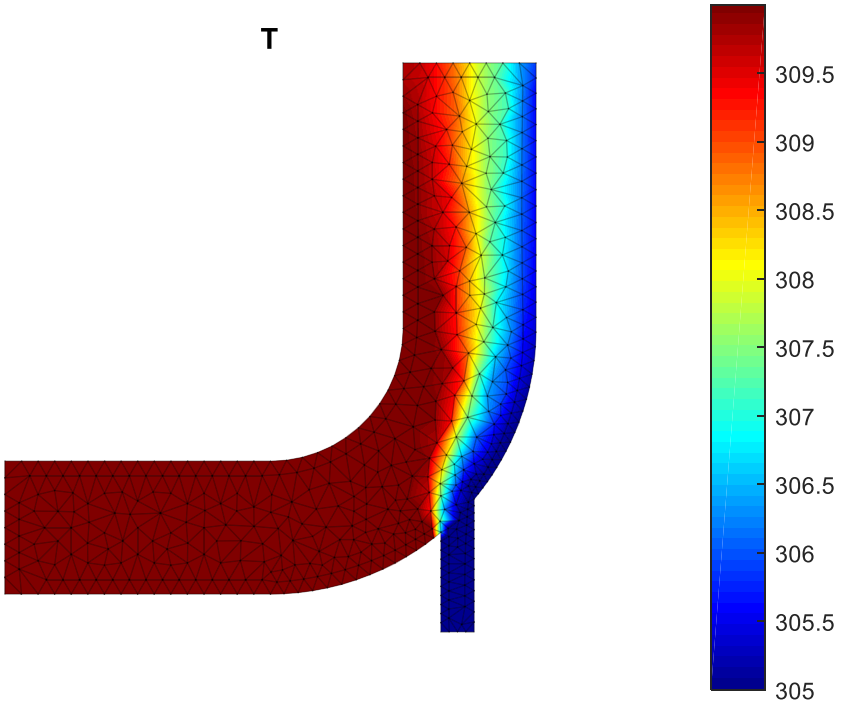


Figure 11 - Temperature contour (k)

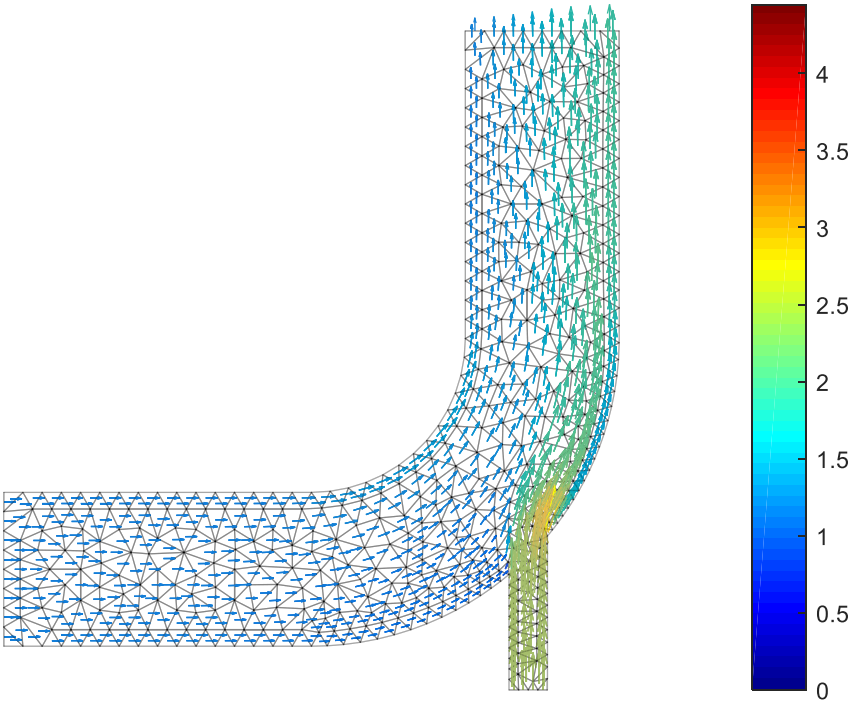
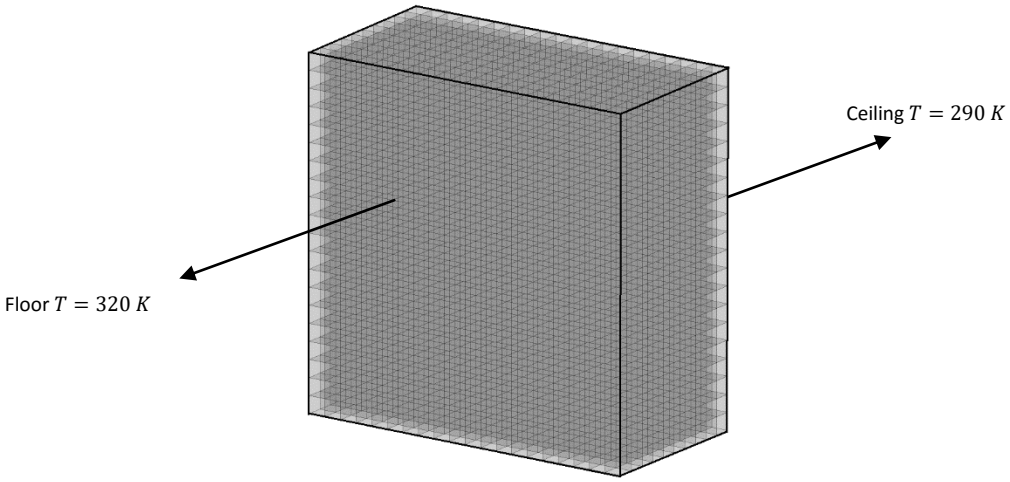


Figure 12 - Velocity vectors

7.3 Heat Transfer

A hot room case will be presented here. A buoyancy driven air flow is simulated in a room which has different temperature values on its floor and ceiling while the walls are adiabatic. The mesh is shown here:



In this problem, Boussinesq approximation is implemented to account for buoyancy effects due to temperature gradients.

The governing equations are:

Momentum:

$$\nabla.(\boldsymbol{vv}) = \nu\nabla^2\boldsymbol{v} + \nabla.\{\nu(\nabla\boldsymbol{v})^T\} - \nabla p - g\beta\left(T - T_{ref}\right)$$

Continuity:

$$\nabla.\boldsymbol{v} = 0$$

Energy:

$$\nabla.(\boldsymbol{v}T) = \alpha\nabla^2 T$$

The corresponding run case is:

```
%--------------------------------------------------------------------------
%
%  written by the CFD Group @ AUB, 2017
%  contact us at: cfd@aub.edu.lb
%==========================================================================
% Case Description:
%     In this test case a hot room is simulated with boussinesq
%     approximation
%--------------------------------------------------------------------------

% Setup Case
cfdSetupSolverClass('heatTransfer');

% Read OpenFOAM Files
cfdReadOpenFoamFiles;

% Setup Time Settings
cfdSetupTime;

% Define new properties
cfdSetupProperty('alpha', 'model', 'nu/Pr');

% Setup Equations
cfdDefineEquation('U', 'div(U*U) = laplacian(nu*U) + div(nu*transp(grad(U))) - grad(p) - g*beta*(T - TRef)'); %
Momentum
cfdDefineEquation('p', 'div(U) = 0'); % Continuity
cfdDefineEquation('T', 'div(U*T) = laplacian(alpha*T)'); % Energy

% Initialize case
cfdInitializeCase;

% Run case
cfdRunCase;
```

Running the case, gives the following velocity field at an arbitrary section plane:

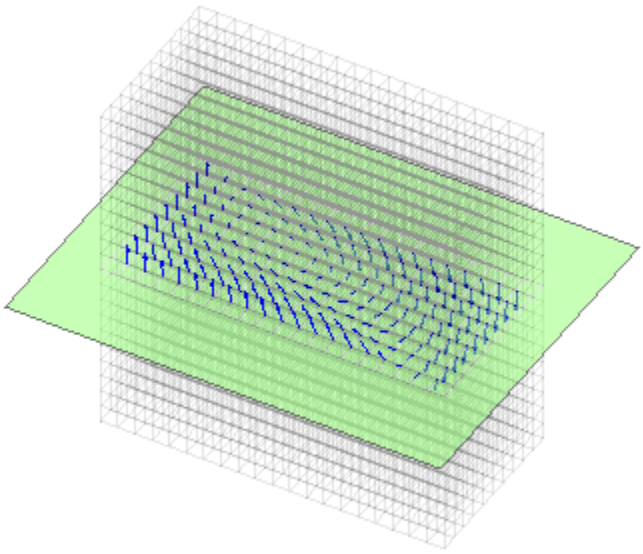


Figure 13 - Velocity field at a section plane