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Python Scripting for Gluing CFD Applications: A Case Study Demonstrating Automation of Grid Generation, Parameter Variation, Flow Simulation, Analysis, and Plotting

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Abstract

One of the simplest yet most useful applications of scripting is the automation of manual interaction with the computer. Here, it means running programs for mesh generation, flow simulation, post–processing analysis, and plotting, and doing it over a complex matrix of initial conditions, boundary conditions, fluid properties, and geometry variants. Python scripting provides the ability to interact with both the operating system and each of the component codes, and to perform complex analysis and plotting.

A case study using OpenFOAM to solve the decaying Taylor–Green vortex, which is an analytical solution to the transient two–dimensional Navier–Stokes equations, is developed. A python script is used to perform a mesh–refinement study for ten different flux–interpolation schemes, and to automatically generate meshes, specify initial conditions, run the flow code, run a custom post-processor which computes solution error in comparison to the benchmark, and create line plots, contour maps, and vector plots. Concluding remarks are provided which summarize readiness for application to ship hydrodynamics, and which identify areas for future work.

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CHAPTER 1

Introduction

1.1 Motivation

Computational fluid dynamics (CFD) has matured to its current status where multiphysics and design-relevant simulations are realizable. Marine engineering examples include integrated design of surface ships, design of marine-propulsors made of advanced materials, and integration of fidelity wake simulations into prediction of ship and submarine acoustic and non-acoustic signatures. However, there are several high–level challenges in performing these simulations. First, the top–level driver/calling program has to see CFD (and the entire "CFD Process") as a modular "black-blox" which can be reliably automated. Second, top–level programs often require large–amounts of fluid dynamics data over a large parameter space. This requires that the driver program manage a matrix of simulations, and resultant data. Third, CFD and other analysis tools (e.g., finite-element analysis), must be coordinated and data must be passed between them. This process is known as code gluing. It is proposed that Python scripting will play an important role in meeting these challenges.

CREATE-Ships has the broad objective to impact acquisition and design of future ships by leveraging high-performance computing. Focus areas include rapid, *and automated*, simulation of hull resistance and associated boundary–layer and free–surface hydrodynamics using fidelity RANS CFD, and development of an Integrated Hydro Design Environment (IHDE) to more tightly couple design and analysis tools. It is envisioned that the IHDE will interface with adjustable–fidelity simulation tools, ranging from empirical databases to potential-flow codes to RANS/DES/LES CFD codes, however, the IHDE will only see the various tools through an interface. Behind this interface, however, is the "CFD Process" which itself is comprised of a number of highly–specialized stand–alone programs.

The Applied Research Lab (ARL) at Penn State University (PSU) is a leader in marine composites and has designed and fabricated numerous composite structures for the U.S. Navy. Current interest is focused on coupling CFD, FEA, and in-house acoustics tools for prediction of fully–coupled fluid–structural–hydroacoustic performance. This is a clear example of a need for code automation and code gluing. Water–tunnel tests of metal and composite hydrofoils are currently being planned/performed as part of student thesis research. The purpose of these tests are to develop understanding and validation databases for fluid-structure interaction (FSI) simulations.

ARL/PSU is also the developer of the Technology Requirements Model (TRM) which is a digital simulation tool for torpedoes. The software supports the full system technology development cycle; i.e., research, design, development, testing, and technology transition to acquisition. TRM's architecture allows for the acoustic interactions (mutual interference) between surface ships, submarines, countermeasures, counter-fire weapons, salvo fired torpedoes, and anti-torpedo torpedoes. However, it lacks the ability to easily incorporate physics–based models of wakes. Current work is focused on integration of CFD into the TRM process, including ships undergoing transient maneuvers. In this case, TRM should be able to either interrogate existing CFD databases, or call a CFD module for development of new data.

From this short list of examples, it should be obvious that there is a large need for improving the interface of CFD to other tools. One of the simplest yet most useful applications of scripting is the automation of manual interaction with the computer. Here, it means running programs for mesh generation, flow simulation, post–processing analysis, and plotting, and doing it over a complex matrix of initial conditions, boundary conditions, fluid properties, material properties, and geometry (hullform, propulsors, etc.) variants. Python scripting provides the ability to interact with both the operating system and each of the component codes, and to perform complex analysis and plotting.

As advertised on the python.org website [1], "Python is a dynamic object-oriented programming language that can be used for many kinds of software development. It offers strong support for integration with other languages and tools, comes with extensive standard libraries, and can be learned in a few days. Many Python programmers report substantial productivity gains and feel the language encourages the development of higher quality, more maintainable code."

There are a number of libraries which greatly extend Python and make it a powerful tool for computational science. Numpy [2] is the fundamental package needed for scientific computing with Python. It contains: a powerful N-dimensional array object; sophisticated broadcasting functions; basic linear algebra functions; basic Fourier transforms; sophisticated random number capabilities; tools for integrating Fortran code; and tools for integrating C/C++ code. Scipy [3] is open-source software for mathematics, science, and engineering. The SciPy library is built to work with NumPy arrays, and provides many user-friendly and efficient numerical routines such as routines for numerical integration and optimization. Together, they run on all popular operating systems, are quick to install, and are free of charge. Matplotlib [4] is a python 2D plotting library which produces publication quality figures in a variety of hardcopy formats and interactive environments across platforms. Matplotlib can be used in python scripts, the ipython shell (in a fashion similar to MATLAB), web application servers, and six graphical user interface toolkits.

An indicator of the importance of python in computational science is the fact that most commercial CFD visualization tools (Ensight, Fieldview, Paraview, Tecplot) are now providing python bindings for controlling the analysis and visualization from a python script. There are also python bindings for MPI (message passing interface) and PETSc (parallel extensible toolkit for scientific computing). Finally, python can interfaced with Fortran and C/C++ by using `f2py` and `swig`, respectively.

With regard to OpenFOAM, there are several python related development activities. The first, is `PyFOAM` [5] which is a library that can be used to: analyze the logs produced by OpenFoam-solvers; execute OpenFoam-solvers and utilities and analyze their output simultaneously; manipulate the parameter files and the initial-conditions of a run in a non-destructive manner; and plots the residuals of OpenFOAM solvers using GNUPLOT. The second is an effort by Hrv Jasak to use `swig` to create python bindings for OpenFOAM libraries. While the latter is in a very preliminary stage, it offers rapid prototyping and debugging, and even easier systems integration.

1.2 Objective

The objective of this report is to demonstrate the use of python scripting for gluing CFD applications. A case study using the decaying Taylor–Green vortex is developed. This problem is an analytical solution to the transient two–dimensional Navier–Stokes equations, and is commonly used for computing the order–of–accuracy of the numerical schemes. [6, 7] A python script is used to perform parameter variation (mesh resolution and convective–scheme flux interpolation), generate meshes, specify initial conditions, run the flow code, run a custom post-processor which computes solution error in comparison to the benchmark, and create line plots, contour maps, and vector plots. Concluding remarks are provided which summarize readiness for application to ship hydrodynamics, and which identify areas for future work.

1.3 Requirements

If you have downloaded the case study tarball, you will need the following software installed on your computer to run the python script:

- `OpenFOAM 1.5.x` [8]
- `python` [1]
- `matplotlib` [4]
- `NumPy` [2]
- `SciPy` [3]

OpenFOAM 1.5.x can be obtained from the OpenCFD `git` repository. Note that this version is source code only, so it will require full compilation. The bug-fix/patched version repository is available at git://repo.or.cz/OpenFOAM-1.5.x.git. The repository can be obtained using the command:

```
[08:54:10][egp@egpMBP:~/OpenFOAM]$git clone git://repo.or.cz/OpenFOAM-1.5.x.git
```

This will create an OpenFOAM-1.5.x directory that the user can subsequently update to the latest published copy using

```
[08:55:05][egp@egpMBP:~/OpenFOAM]$git pull git://repo.or.cz/OpenFOAM-1.5.x.git
```

While it is not required, `iPython` [9] is nice to have since it permits interactive running of the script. It gives an interface similar to `MATLAB`.

CHAPTER 2

Case Study

2.1 Python Scripting

To meet the goals of the multi-physics examples previously mentioned, an approach needs to be developed where fidelity CFD simulations can be performed rapidly and automatically, and where data is returned back to a driver code (e.g., IHDE) for integration in the design/analysis cycle. A notional flow chart to accomplish this is shown in figure 2.1. This flow chart shows iterative loops over hullform geometry, ship speed, and mesh refinement (all of w. Inside the loops is the typical CFD Process: mesh generation; setting of initial conditions, boundary conditions, and fluid properties; flow solution; analysis; and plotting and visualization.

Instead of using a practical surface–ship example for the case study, a simplified problem was chosen so that it would run fast (i.e., a few minutes on a laptop), and be easy to distribute by email or website download. The flow chart for the case study of the Taylor–Green vortex problem is shown in figure 2.2. It is nearly identical to the flow chart for the ship, except for the iteration loops are over the type of flux interpolation scheme `divScheme` and mesh refinement. Also, several other utilities are used: `funkySetfields`, and `analyticalSolutionTaylorVortex`.

The python script `runScript.py` for the case study is located in the root of the tarball. It is 190 lines long, and could be greatly shortened with definition of a few functions or classes/members. It is executed at the command line with the command

```
[16:10:39][egp@TaylorVortex]$ ./runScript.py
```

The script loops over 4 meshes, and 10 `divScheme` represented by the python lists

```
meshDir = ['mesh8', 'mesh16', 'mesh32', 'mesh64']

divSchemes=[ 'linear', 'cubic', 'downwind', 'midPoint', 'MUSCL',
             'Minmod', 'QUICK', 'filteredLinear', 'upwind', 'vanLeer']
```

The loops are executed using the python `for` loop, e.g.,

```
for mesh in meshDir:
        meshIndex =meshDir.index(mesh)
        # further processing on mesh
```

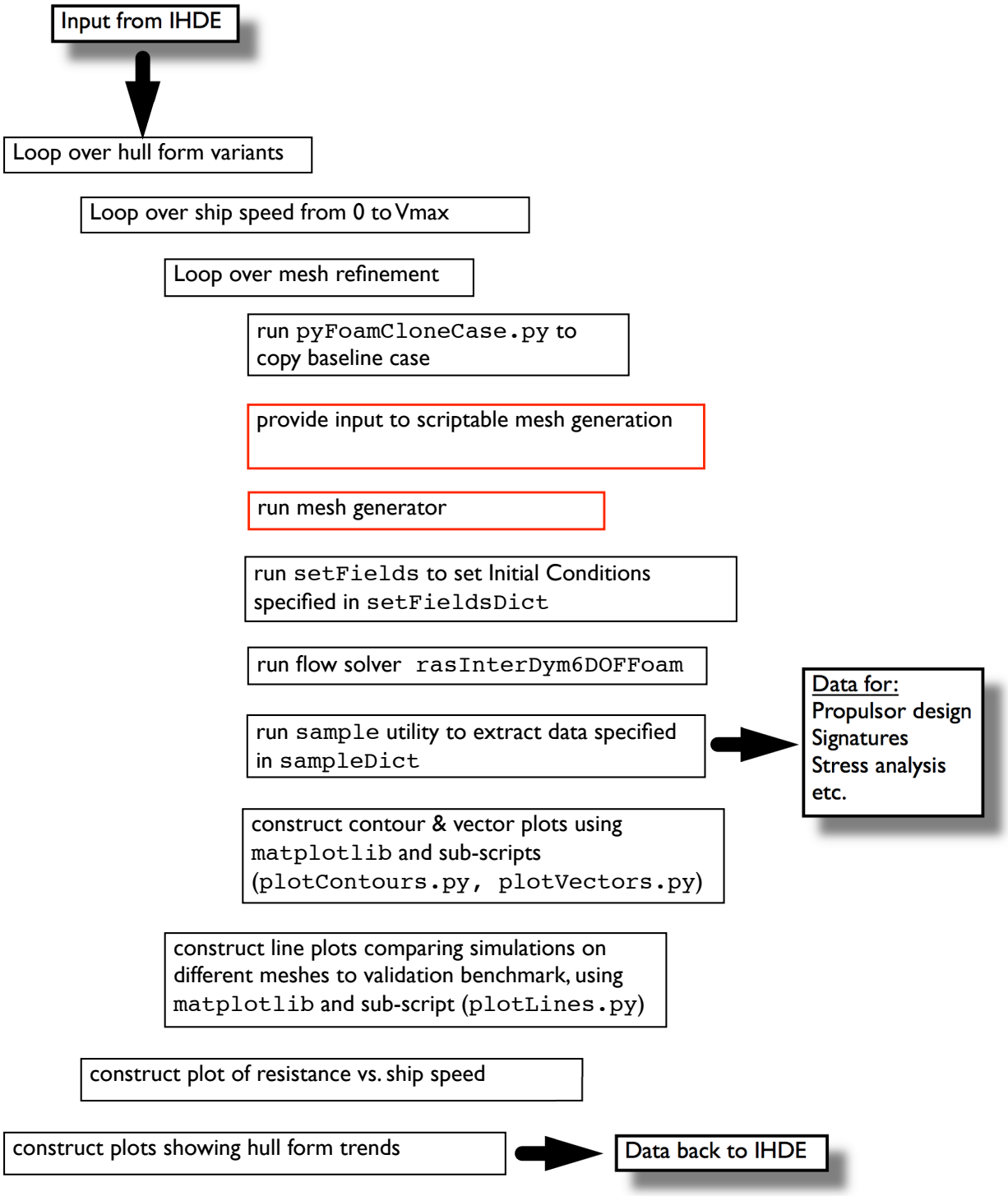


Figure 2.1: Flow Chart of a Notional Python Script for Controlling Ship Hydrodynamics Simulations

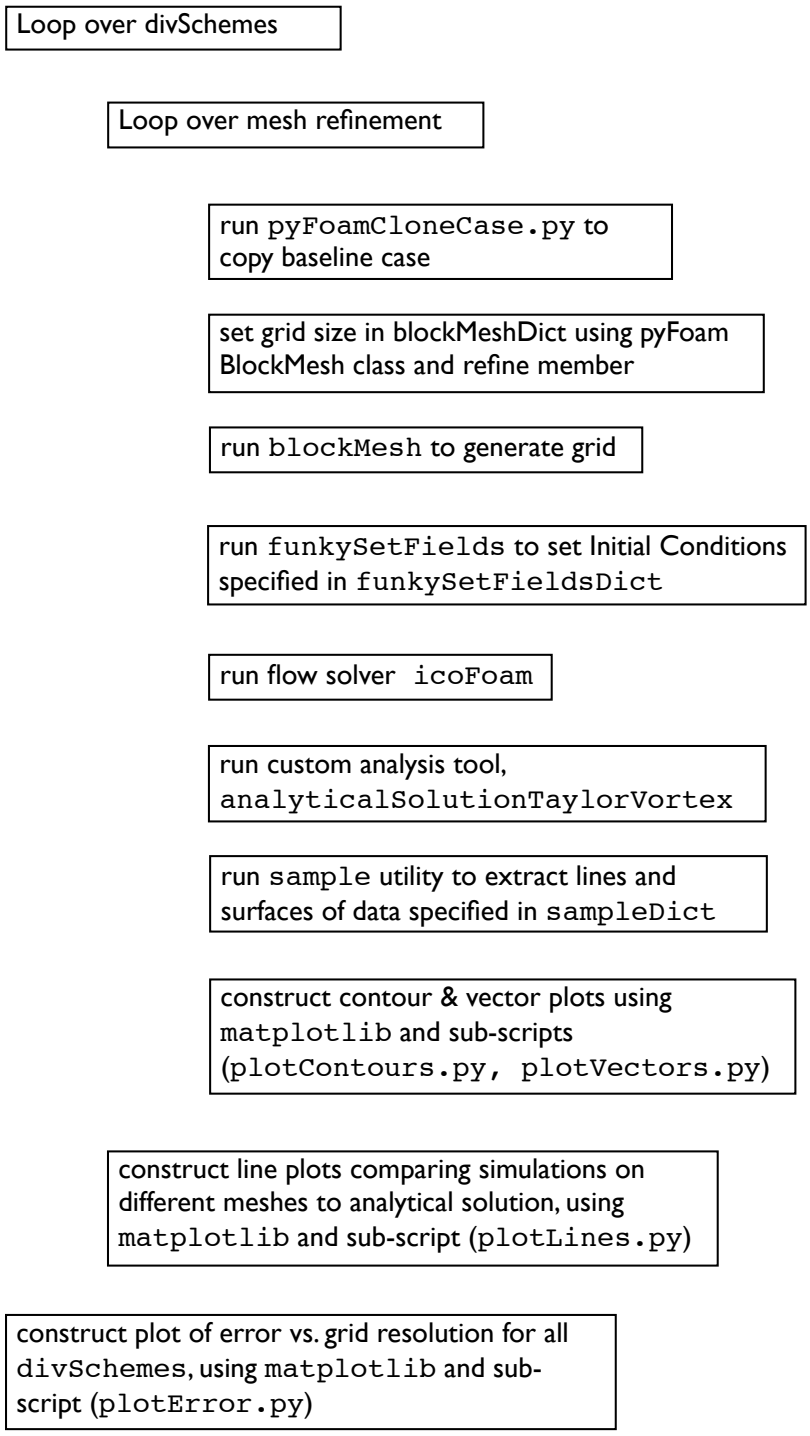


Figure 2.2: Flow Chart of a Python Script for Controlling Simulations of Taylor Vortex

2.2 Analytical Benchmark: 2D Taylor-Green Vortex

The 2D Taylor-Green Vortex is an analytical solution to the Navier–Stokes equations, and has long been used for testing and validation of temporal and spatial accuracy of the numerical scheme. [6, 7, 10, 11].

In the domain $-\frac{\pi}{2} \leq x, y \leq \frac{\pi}{2}$, the solution is given by

$$u = \sin x \cos y F(t) \qquad v = -\cos x \sin y F(t) \tag{2.1}$$

where $F(t) = e^{-2\nu t}$, ν being the kinematic viscosity of the fluid. The pressure field p can be obtained by substituting the velocity solution in the momentum equations and is given by

$$p = \frac{\rho}{2} (\cos 2x + \sin 2y) F^2(t) \tag{2.2}$$

Equations 2.1 and 2.2 are used to prescribe the initial conditions at time = 0. Figure 2.3, which shows velocity vectors, velocity–magnitude contours, and pressure contours, illustrates the solution at time = 1.0, for the case where $\nu = 1.0 m^2/s$. The velocity field has odd-symmetry and the pressure-field is periodic in x and y directions. This information is used in assigning boundary conditions. Symmetry conditions are applied on all boundaries (except for the empty faces in the z-direction).

2.3 Use of PyFoam

Referring back to figure 2.2, the first steps inside the loop are to clone the baseline case and to refine the mesh. For both of these steps, the pyFoam utilities [5] are utilized.

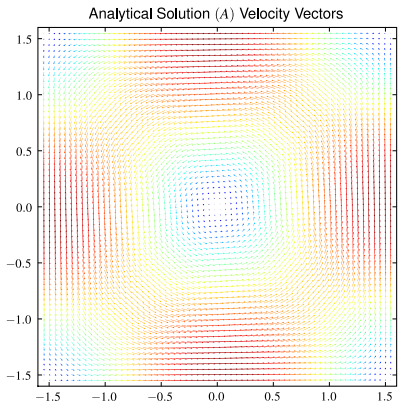
`pyFoamCloneCase.py` is a `pyFoam` application which creates a copy of a case with only the most essential files (`0, constant, system` directories). It has two command line arguments: the source case (`../../baseline`) and the destination case (`mesh`, where `mesh` is a list member which refers to the mesh resolution). In the text that follows, which is from `runScript.py`, the string `cmd` is passed to the `call` member of the `subprocess` module.

```
# use pyFoam to clone the baseline case
cmd='pyFoamCloneCase.py ../../baseline %s' % mesh
pipefile = open('output', 'w')
retcode = call(cmd,shell=True,stdout=pipefile,stderr=pipefile)
pipefile.close()
os.remove('output')
```

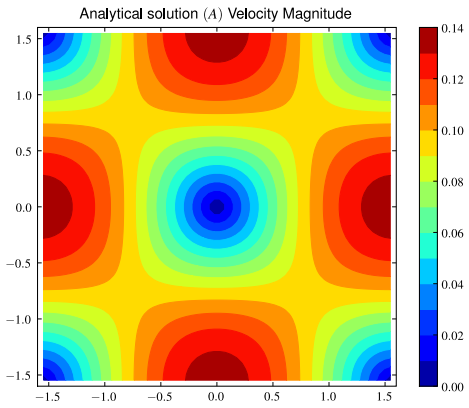
The `subprocess` module allows you to spawn processes, connect to their input/output/error pipes, and obtain their return codes. `cmd` is passed to the shell using the short cut function `call` which runs the command with arguments, waits for command to complete, and then returns the `returncode` attribute. It is used to run all of the component codes in the CFD Process.

2.4 Mesh Generation

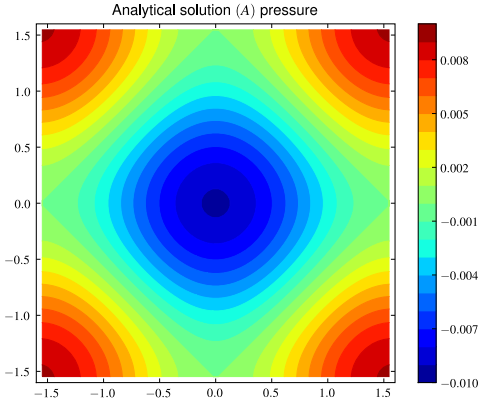
Since one of the loops is to iterate over mesh resolution (8x8, 16x16, 32x32, 64x64), the input to the mesh generation tool needs to be modified inside the script. In this simple case, the OpenFOAM mesher `blockMesh` is used. It reads a dictionary `constant/polymesh/blockMeshDict` and generates a hex mesh using algebraic methods. In the script `runScript.py`, the `pyFoam` class



(a) Velocity Vectors



(b) Velocity Magnitude Contours



(c) Pressure Contours

Figure 2.3: Analytical Solution for the Taylor–Green Vortex Problem at time = 1

```
# set block size in blockMeshDict
dict=‘‘constant/polyMesh/blockMeshDict’’        # blockMeshDict
bm=BlockMesh(dict)                              # define bm to be a pyFoam BlockMesh object
number=meshDir.index(mesh)                      # find index of current mesh: 0, 1, 2, 3
bm.refineMesh\left( 2**number,2**number,1))     # refineMesh by factor of 2^number over baseline
meshDim = 8*2**number
```

A (`BlockMesh`) object and member (`refineMesh`) are used to change the values in `blockMeshDict`. The `blockMesh` utility is run with the `subprocess.call` function.

```
# run blockMesh
cmd='blockMesh'
pipefile = open('output', 'w')
retcode = call(cmd,shell=True,stdout=pipefile)
pipefile.close()
os.remove('output')
```

2.5 Variation of the `divScheme`

When looping over the `divSchemes` list, the `system/fvSchemes` dictionary has to be modified with the `divScheme` of the current iteration. `pyFoam` has a series of utilities for modifying dictionaries. At the time of writing this report, `pyFoamWriteDictionary.py` was not able to process the string ‘‘`div(phi,U)`’’. Therefore, a small piece of python code was written to read the dictionary, search for ‘‘`div(phi,U)`’’, and replace the `divScheme` with the value of the current iteration. The code in `runScript.py` responsible for this is listed below.

```
# change the divScheme for ‘‘div(phi,U)  Gauss linear;’’ in the fvSchemes file
infilename='system/fvSchemes'
outfilename='system/fvSchemesTemp'
ifile = open( infilename, 'r')
ofile = open(outfilename, 'w')
lines = ifile.readlines()
for line in lines:
       words = line.split()
       for word in words:
              index = words.index(word)
              if word ==  'div(phi,U)':
                     words[index+2] = divScheme+';'
                     continue
       newline=' '.join(words)
       ofile.write('%s\n' % newline)
ifile.close()
ofile.close()
os.remove(infilename)
os.rename(outfilename,infilename)
```

2.6 Initial Conditions: funkySetFields

The `funkySetFields` utility of Gschaider [12] is used to prescribe the initial conditions from the analytical solution in equations 2.1 and 2.2. `funkySetFields` was designed to set the value of a scalar or a vector field depending on an expression that can be entered via the command line or a dictionary. It can also be used to set the value of fields on selected patches or set non-uniform initial-conditions without programming. It has been described as the OpenFOAM `setFields` utility on steroids.

To use the analytical solution as the initial conditions, the following text is inserted into the dictionary `system/funkySetFieldDict`.

```
expressions
 (
        TaylorVortexVelocity
        {
                field U;
                expression ‘‘vector( -cos(pos(.x)*sin(pos(.y)),
                                    (sin(pos(.x)*cos(pos(.y)),
                                    0)’’;
        }
        TaylorVortexPressure
        {
                field p;
                expression ‘‘-0.25*(cos(2.*pos(.x)+cos(2.*pos(.y))’’;
        }
 );
```

As with the other component programs, `funkySetFields -time 0` is sent to the shell using the subprocess.call function. The portion of `runScript.py` which executes this utility is listed below.

```
#run funkySetFields to set initial conditions
cmd='funkySetFields -time 0'
pipefile = open('output', 'w')
retcode = call(cmd,shell=True,stdout=pipefile)
pipefile.close()
os.remove('output')
```

2.7 Flow Solver: icoFoam

Since the Taylor-Green vortex is a transient, laminar flow problem, the `icoFoam` solver is used to solve for velocity and pressure fields. `icoFoam` solves the incompressible laminar Navier-Stokes equations using the PISO algorithm which is a time-accurate algorithm requiring initial and boundary conditions. The `icoFOAM` solver reads the following dictionaries: `system/controlDict`, `system/fvSchemes`, `system/fvSolution`, `constant/transportProperties`. Details of the icoFoam solver are provided in the Appendices.

In the `runScript.py` script, the flow code is executed with the following commands.

```
# run icoFoam to solve Navier Stokes equations
cmd='icoFoam > log 2>&1'
pipefile = open('output', 'w')
retcode = call(cmd,shell=True,stdout=pipefile)
pipefile.close()
os.remove('output')
```

2.8 Solution Post–Processing

Solution post–processing includes manipulation of data, comparison of simulation and benchmark (which, in this case, is an analytical solution), and plotting. The following sections will explain the post–processing, and present some of the results.

2.8.1 Error Computation: analyticalSolutionTaylorVortex

The easiest way to compute error $E = S - A$, where S is the simulation result and A is the analytical solution, is to write a custom OpenFOAM utility which can access the various OpenFOAM data structures. For the case study, `analyticalSolutionTaylorVortex` was written and is located in the `tools` directory. It reads the mesh and simulation results, computes the analytical solution at the cell centers, and calculates the error E. It is compiled with the standard OpenFOAM `wmake` machinery. The following code from `runScript.py` shows that the utility is run with the `subprocess.call` function, and that `stdout` is written to the `pipefile` named `ASTVOutput`. Then, the script parses this file and searches for the strings `'Maximum'` and `'Average'`. After these strings are found, the value of `maxError` and `aveError` are read and held in memory for plotting.

```
# run custom post-processor for computing analytical solution at each time step,
# and for computing comparison error
cmd='analyticalSolutionTaylorVortex -time 1'
pipefile = open('ASTVOutput', 'w')
retcode = call(cmd,shell=True,stdout=pipefile)
pipefile.close()

# extract maximum error at endTime (time = 1) from STDOUT
pipefile = open('ASTVOutput', 'r')
lines = pipefile.readlines(
for line in lines:
        words = line.split()
        for word in words:
              if word == 'Maximum':
                    value=float(words[len(words)-1])
                    maxError.append(value)
              if word == 'Average':
                    value=float(words[len(words)-1])
                    aveError.append(value)
pipefile.close()
```

2.8.2 Solution sampling

Solution sampling is accomplished using the OpenFOAM utility `sample`, which reads the dictionary `system/sampleDict`. It is executed by the shell using the `call` function.

```
# run sample utility
cmd='sample -time 1'
pipefile = open('output', 'w')
retcode = call(cmd,shell=True,stdout=pipefile)
pipefile.close()
os.remove('output')
```

2.8.3 Contour Maps and Vector Plots

Contour maps and vector plots are created using `matplotlib` [4]. The `runScript.py` calls two sub-scripts, `tools/plotContours.py` and `tools/plotVectors.py`. These sub-scripts expect 3 command-line arguments, which are used primarily for naming the plot files. After creation, the plot files are moved to a directory in the root of the case study named `figures`.

```
# construct contour & vector plots
cmd='python ../../../tools/plotContours.py '+ str(meshDim)+' '+divScheme+' '+mesh
pipefile = open('output', 'w')
retcode = call(cmd,shell=True,stdout=pipefile)
```

```
pipefile.close()
os.remove('output')

cmd='python ../../../tools/plotVectors.py '+ str(meshDim)+' '+divScheme+' '+mesh
pipefile = open('output', 'w')
retcode = call(cmd,shell=True,stdout=pipefile)
pipefile.close()
os.remove('output')

# move pdf image files to figures directory
filelist=glob.glob('*.pdf')
for file in filelist:
        shutil.move(file, origdir+``/figures/.'')
```

Figure 2.4 shows contours of velocity magnitude and pressure, for the four different meshes. In this case, the solutions all used the upwind scheme for the convective terms in the Navier-Stokes equations.

Figure 2.5 shows the comparison error $E = S - A$ on the fine mesh for each of the convective schemes. Here, it can be seen that the first–order schemes (upwind, downwind) have the largest errors (on the order of 1%).

2.8.4 Grid Studies: Point–Data Comparison

Detailed point–data comparisons are made along a sampling line which corresponds to $y = 0$. These plots were created by using the `plotLines.py` sub-script and the following code in `runScript.py`.

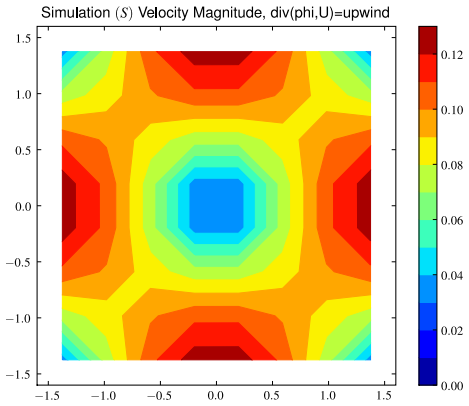
```
# construct line plots comparing all meshes for a given divScheme
cmd='python ../../tools/plotLines.py '+divScheme
pipefile = open('output', 'w')
retcode = call(cmd,shell=True,stdout=pipefile)
pipefile.close()
os.remove('output')
filelist=glob.glob('*.pdf')
for file in filelist:
       shutil.move(file, origdir+``/figures/.'')
```

Figure 2.6 shows a comparison of velocity and pressure to the analytical solution for each `divScheme` and for each mesh.

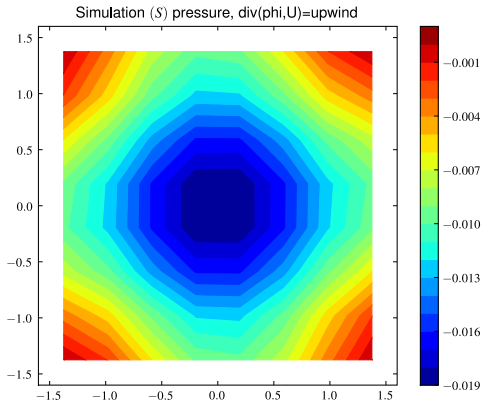
2.8.5 Grid Studies: Average Error vs. Mesh Refinement

The last plot is to extract global data from each simulation and compute and plot average error over the domain, as a function of grid resolution. This is accomplished by running the subscript `plotError.py`. The snippet of code from `runScript.py` that performs this step is listed below.

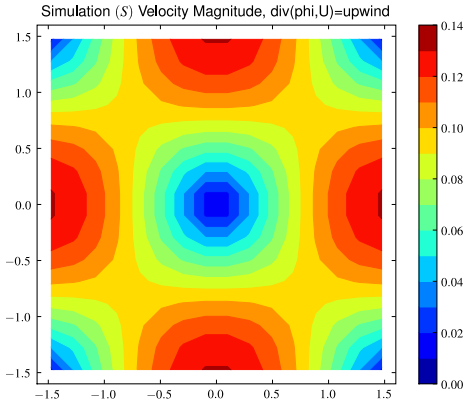
```
cmd='python ../tools/plotError.py'
pipefile = open('output', 'w')
retcode = call(cmd,shell=True,stdout=pipefile)
pipefile.close()
os.remove('output')
filelist=glob.glob('*.pdf')
for file in filelist:
        shutil.move(file, origdir+``/figures/.'')
```



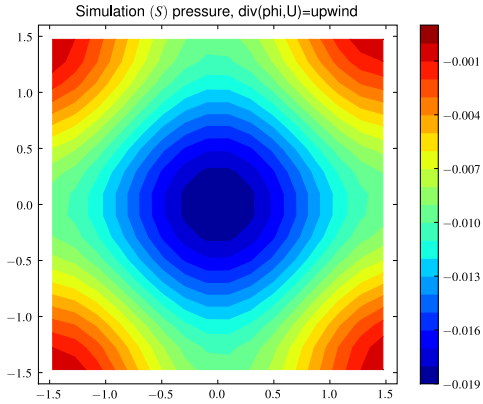
(a) 8x8, velocity



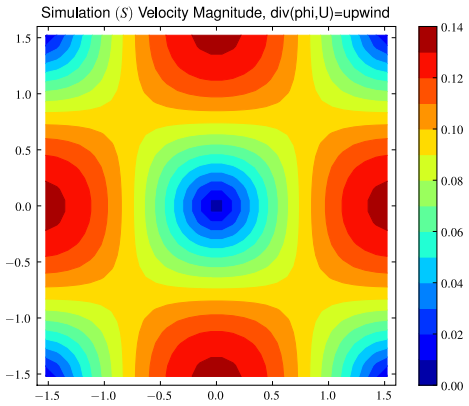
(b) 8x8, pressure



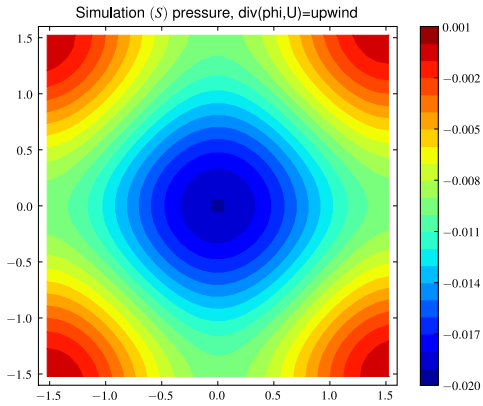
(c) 16x16, velocity



(d) 16x16, pressure

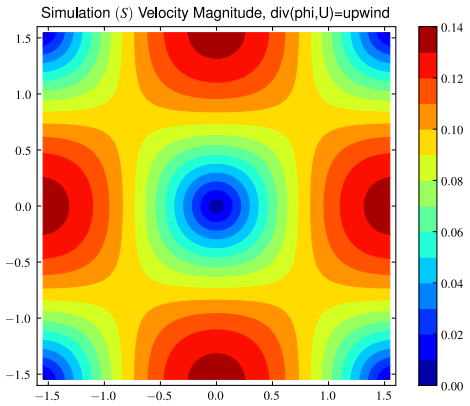


(e) 32x32, velocity

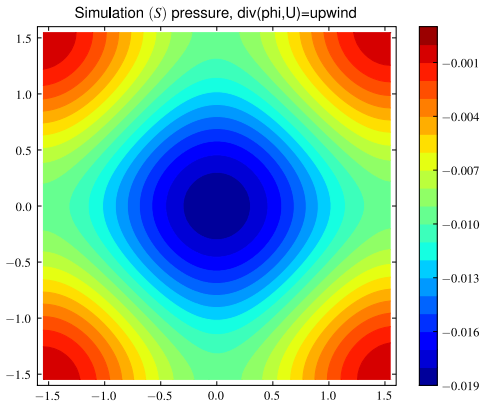


(f) 32x32, pressure

Figure 2.4: Typical Solution Convergence with Mesh Refinement.



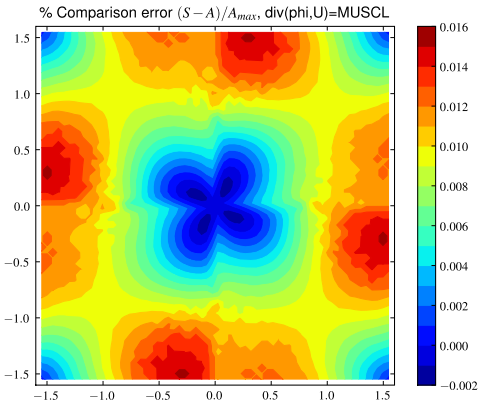
(g) 64x64, velocity



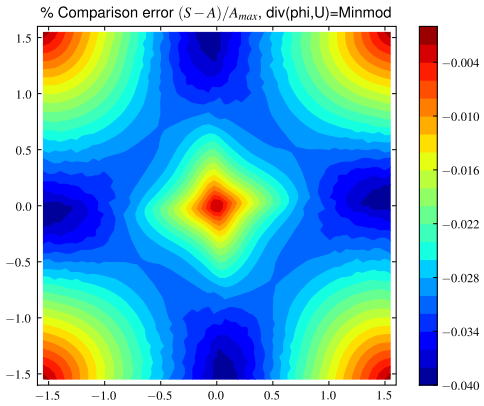
(h) 64x64, pressure

Figure 2.4: Typical Solution Convergence with Mesh Refinement, continued.

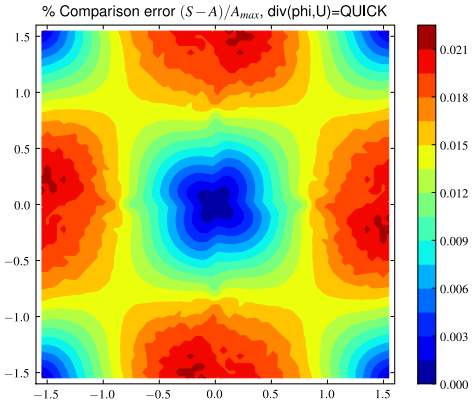
Figure 2.7 shows the result of this analysis. In this plot, the comparison error E is normalized by the maximum velocity magnitude in the domain. This is plotted again the grid resolution normalized by the fine grid Δx. This means that $\frac{\Delta x}{\Delta x_{finest}} = 1,2,4,8$ correspond to the finest, fine, medium, and coarse grids, respectively. The plot in Figure 2.7 shows that the 1st–order schemes (upwind, downwind) have lower rate of grid convergence, whereas the remaining 2nd–order schemes have the same slopes, but with different absolute errors. It should be noted that all simulations were performed with the 2nd-order temporal scheme, `CrankNicholson`, and with a `maxCo` $= 0.1$. This means that the Δt is reduced as the grid is refined, and that Figure 2.7 is a measure of both overall temporal and spatial error.



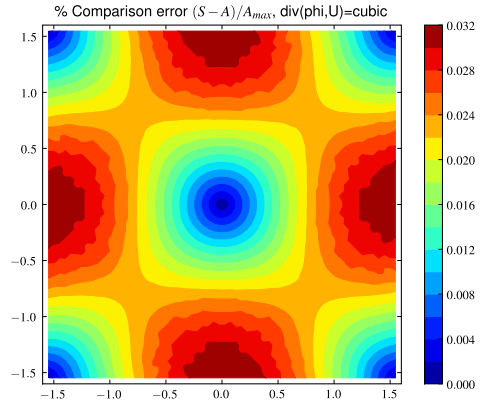
(a) MUSCL



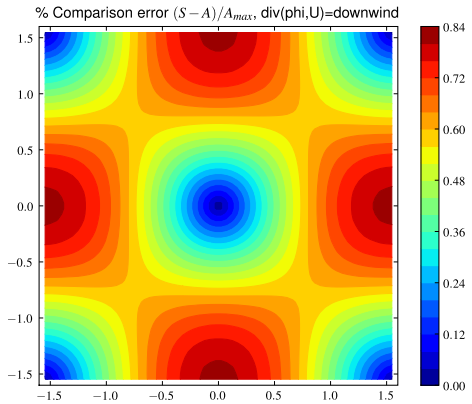
(b) Minmod



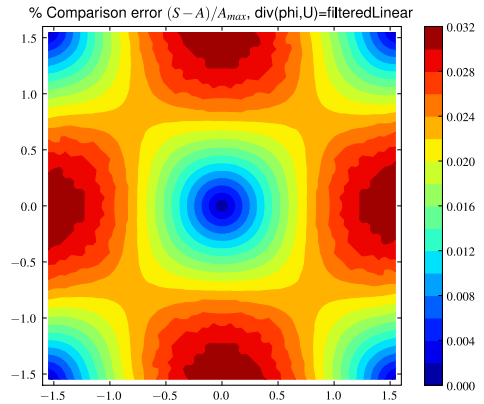
(c) QUICK



(d) cubic

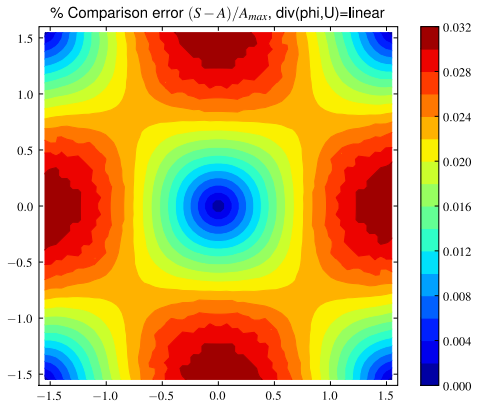


(e) downwind

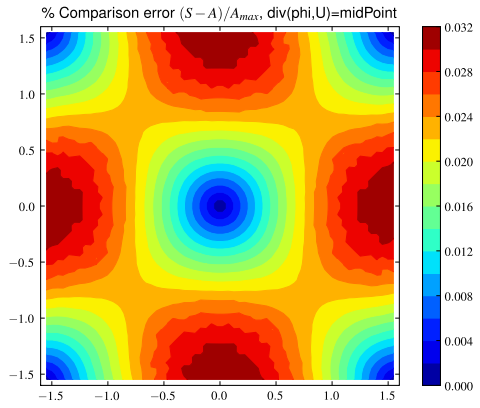


(f) filteredLinear

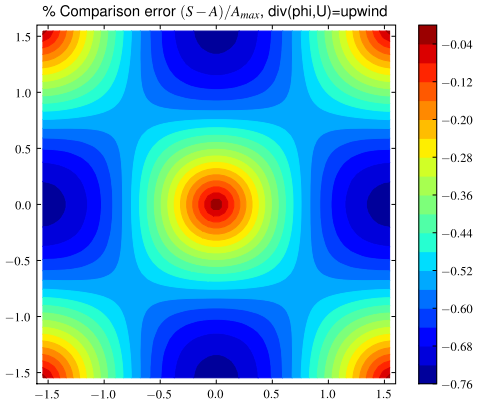
Figure 2.5: Velocity–Magnitude Comparison Error $E = S - A$ on (64x64) Mesh for Each Scheme



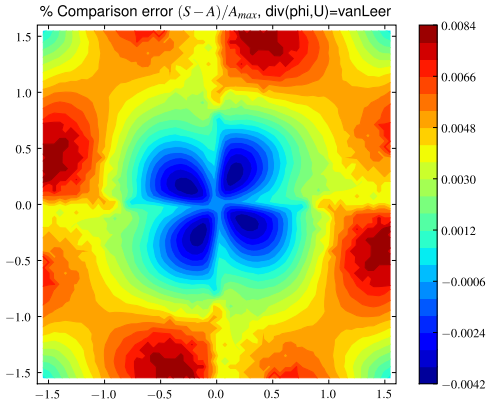
(g) linear



(h) midPoint

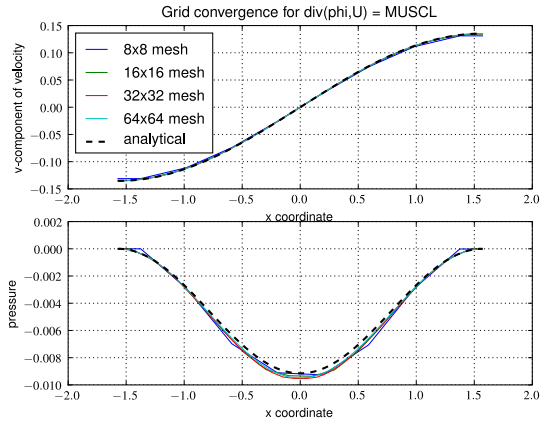


(i) upwind

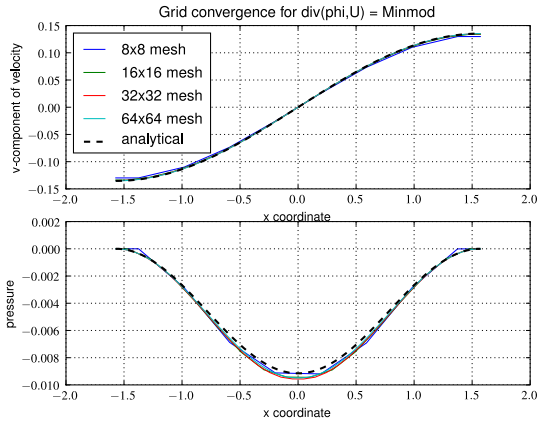


(j) vanLeer

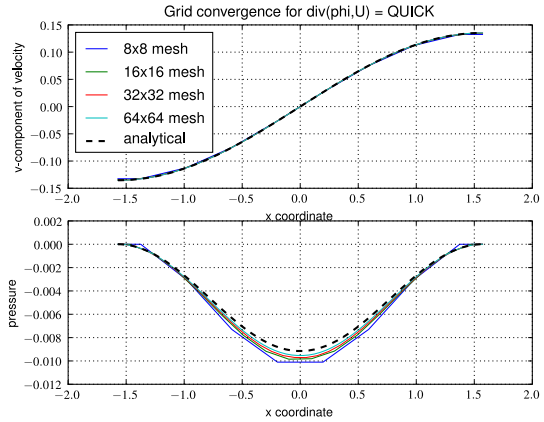
Figure 2.5: Velocity–Magnitude Comparison Error $E = S - A$ on (64x64) Mesh for Each Scheme, continued



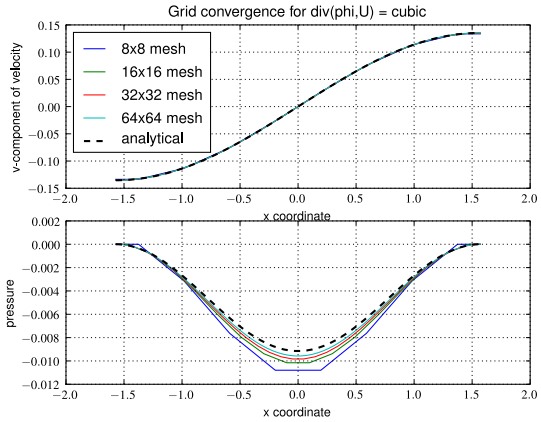
(a) MUSCL



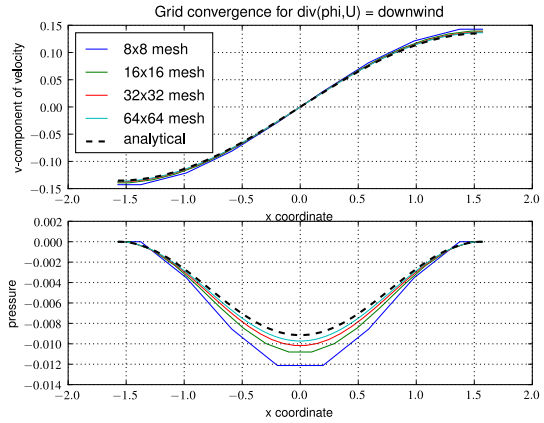
(b) Minmod



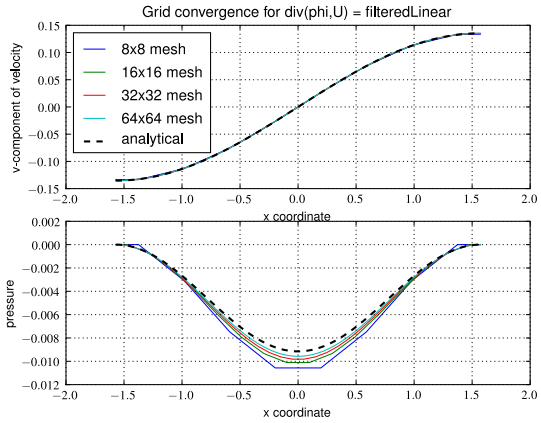
(c) QUICK



(d) cubic

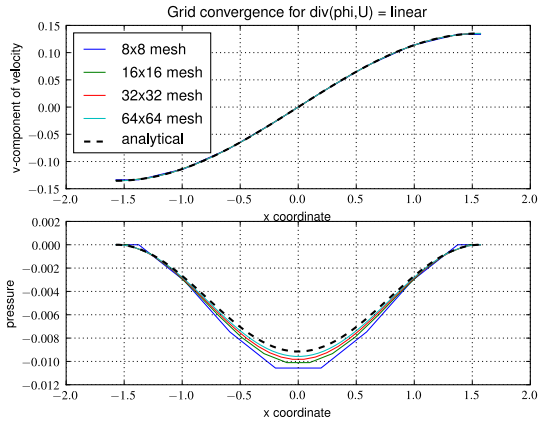


(e) downwind

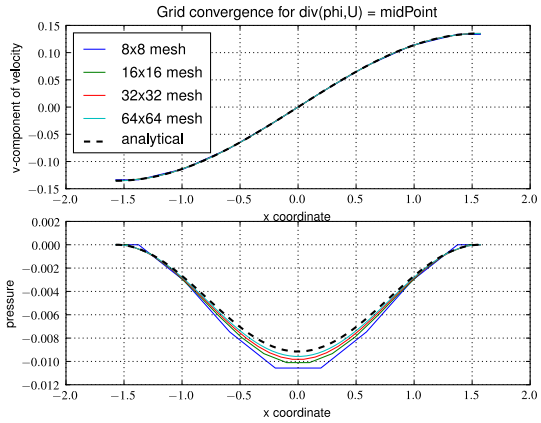


(f) filteredLinear

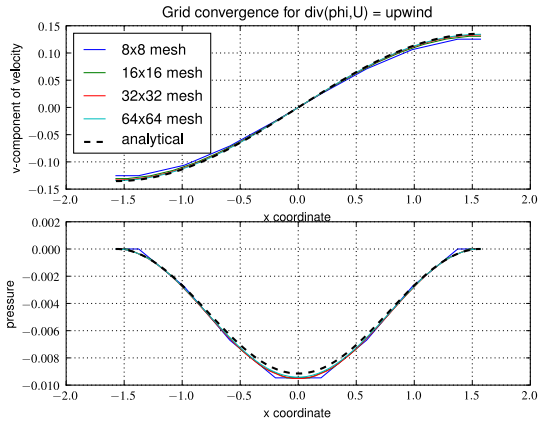
Figure 2.6: Comparison of Velocity and Pressure to Analytical Solution.



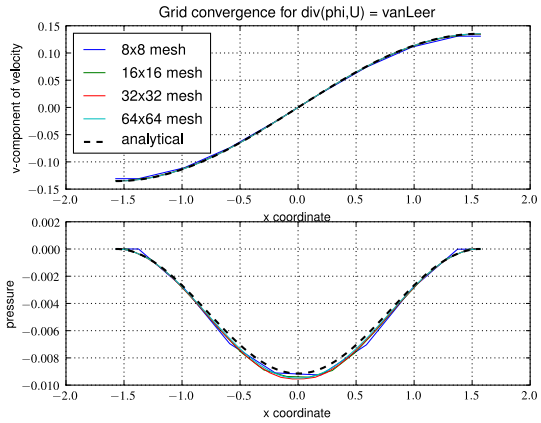
(g) linear



(h) midPoint



(i) upwind



(j) vanLeer

Figure 2.6: Comparison of Velocity and Pressure to Analytical Solution, continued.

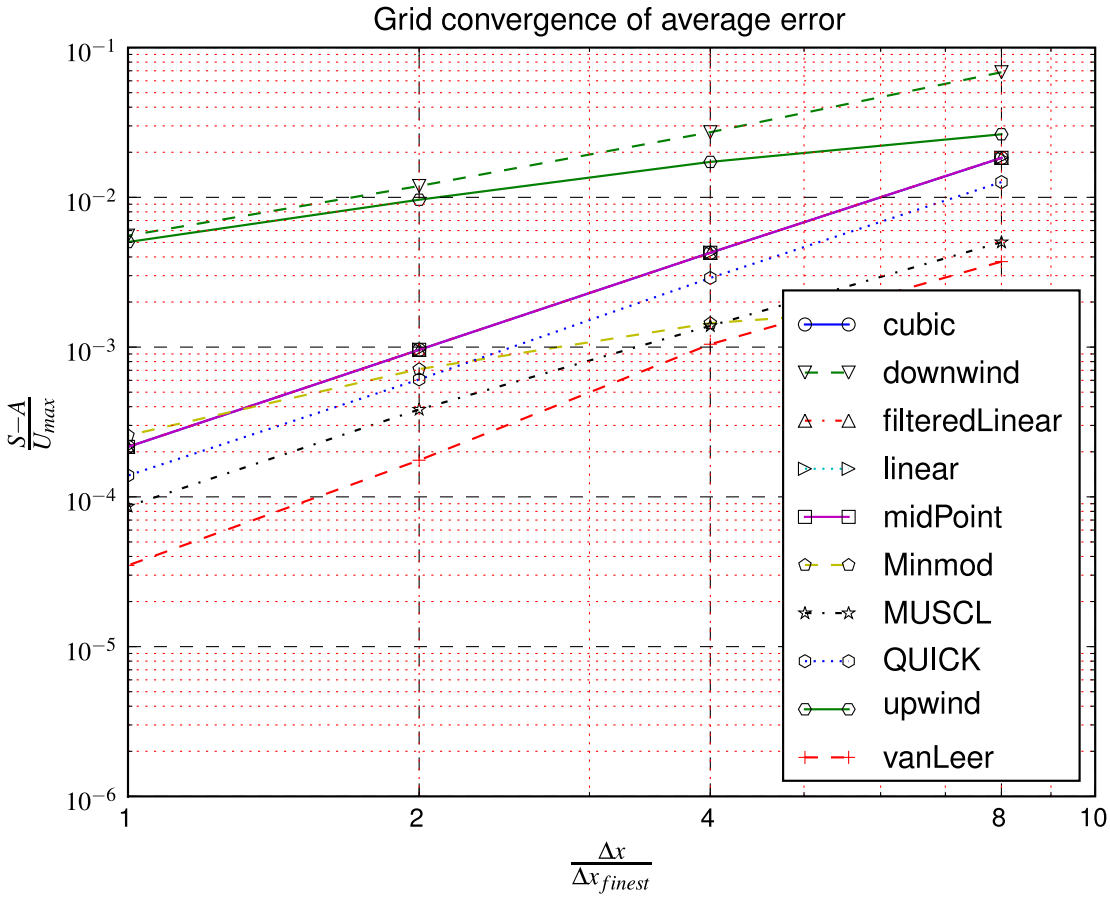


Figure 2.7: Average Error vs. Grid Resolution for Different `divScheme`.

CHAPTER 3

Concluding Remarks

In this report, a case study demonstrating the use of python for code gluing was developed. A python script was used to perform a mesh–refinement study for ten different flux–interpolation schemes, and to automatically generate meshes, specify initial conditions, run the flow code, run a custom post-processor which computes solution error in comparison to the benchmark, and create line plots, contour maps, and vector plots.

For certain classes of problems, the approach is fully ready for application to ship hydrodynamics. These problems include simple geometries, and problems where grid generation can be performed prior to CFD simulation. This is due to the fact that automated, and robust, mesh generation for complex ship hullforms is currently not possible. Possible solutions which need to be further investigated are: use and improvement of hex-dominant meshing techniques such as Harpoon and snappyHexMesh; use of Gridgen in batch–mode with Pointwise Glyph scripting; and testing of NASA Ames approach of scripting overset meshes with hyperbolic near field, and box-mesh far-field [13]. In addition, CREATE has an infrastructure component with the goal of developing more automated grid generation capabilities. As progress is made on this front, the ability to fully automate the CFD process for complex geometries will improve.

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APPENDIX A

OpenFOAM Solver: icoFoam

In following Appendices, details on the numerical methods used in icoFoam are presented. Most of the material has been directly extracted from Hrv Jasak's PhD thesis [14], OpenCFD User and Programmers Guides [15,16], and the OpenFOAM Wiki http://openfoamwiki.net/index.php/IcoFoam.

A.1 Incompressible Navier-Stokes Equations

The 2D incompressible Navier-Stokes equation in the absence of body force is given by

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{A.1}$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) \tag{A.2}$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial y} + \nu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) \tag{A.3}$$

where equations A.1 and A.2–A.3 represent the conservation of mass and linear momentum, respectively.

A.2 Finite Volume Discretization

The governing equations for conservation of mass, conservation of momentum, and transport of scalars can be represented by the generic transport equation for ϕ

$$\frac{\partial \rho\phi}{\partial t} + \nabla\cdot(\rho\mathbf{U}\phi) - \nabla\cdot(\rho\Gamma_\phi\nabla\phi) = S_\phi(\phi) \tag{A.4}$$

which is comprised of 4 basic terms: temporal acceleration; convective acceleration; diffusion; and a source term. The finite volume method requires that each term in Eq. (A.4) be satisfied over

the control volume V_p around the point P in the integral form

$$\int_t^{t+\Delta t} \left[\frac{\partial}{\partial t} \int_{V_p} \rho\phi \, dV + \int_{V_p} \nabla \cdot (\rho \mathbf{U}\phi) \; dV - \int_{V_p} \nabla \cdot (\rho \Gamma_\phi \nabla \phi) \; dV \right] dt = \int_t^{t+\Delta t} \left[\int_{V_p} S_\phi \left(\phi \right) \; dV \right] dt \tag{A.5}$$

The discretization of each term will be discussed in the following sections.

A.2.1 Spatial Discretization

The solution domain is discretized into computational cells, or finite volumes, on which the governing equations are discretized, reduced to algebraic form, and solved with numerical methods. As shown in Figure (A.1), OpenFOAM is based upon general polyhedral cells. The cells are contiguous, i.e., they do not overlap one another and completely fill the domain. Dependent variables and other properties are principally stored at the cell centroid P, although they may be stored on faces or vertices. The cell is bounded by a set of faces, given the generic label f. Since the mesh can be a general polyhedral, there is no limitation on the number of faces bounding each cell, nor any restriction on the alignment of each face.

The first step in spatial discretization is to transform the volume integrals in Eq. (A.5) to surface integrals by using Gauss's Theorem (also known as the Divergence theorem). In it's most general form, Gauss's Theorem can be written as

$$\int_V \nabla \star \phi \, dV = \int_S d\mathbf{S} \star \phi \tag{A.6}$$

where $\mathbf{S}$ is the surface area vector, ϕ represents any tensor field, and the star operator $\star$ is used to represent any tensor product, i.e., inner, outer, cross and the respective derivatives (div, grad, curl). Volume and surface integrals are then linearized using appropriate schemes which are described for each term.

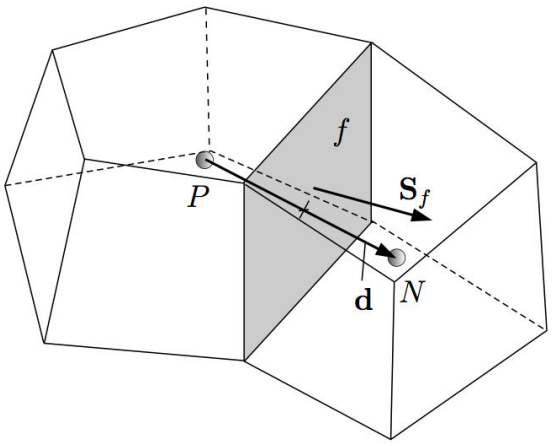

Figure A.1: Parameters in finite volume discretization

Convection Term

The convection term is integrated over a control volume and linearized as follows:

$$\int_V \nabla \cdot (\rho \mathbf{U} \phi)\, dV = \int_S d\mathbf{S} \cdot (\rho \mathbf{U} \phi) = \sum_f \mathbf{S}_f \cdot (\rho \mathbf{U})_f \, \phi_f = \sum_f F \phi_f \tag{A.7}$$

where the face field ϕ_f can be evaluated using a variety of schemes including central, upwind, and blended differencing. Central (or linear) differencing, which is second-order accurate, can be written as:

$$\phi_f = f_x \phi_P + (1 - f_x)\, \phi \tag{A.8}$$

$$f_x = \frac{\overline{fN}}{\overline{PN}} \tag{A.9}$$

OpenFOAM also includes two other centered schemes: cubicCorrection and midPoint. Upwind differencing for ϕ_f, which guarantees boundedness but is first-order accurate, can be written as

$$\phi_f = \begin{cases} \phi_P & \text{for} \quad F \geq 0 \\ \phi_N & \text{for} \quad F < 0 \end{cases} \tag{A.10}$$

In addition to the standard upwind scheme, linearUpwind, skewLinear and Quick schemes are variants of upwinded schemes which are available in OpenFOAM. Finally, there are a number of blended schemes which attempt to preserve both boundedness and accuracy of the solution. The gamma scheme can be written as

$$\phi_f = (1 - \gamma)\, (\phi_f)_{UD} + \gamma\, (\phi_f)_{CD} \tag{A.11}$$

where the blending factor $0 \leq \gamma \leq 1$ determines how much dissipation is introduced.

The mass flux F in Eq. (A.7) is calculated from interpolated values of ρ and $\mathbf{U}$. Similar to interpolation of ϕ_f, F can be evaluated using a variety of schemes including centered, upwinded, and blended schemes, the latter of which includes a number of TVD/NVD schemes (such as limitedLinear, vanLeer, MUSCL, limitedCubic, SFCD, and Gamma).

Laplacian Term

The Laplacian term is integrated over a control volume and linearized as follows:

$$\int_V \nabla \cdot (\Gamma \nabla \phi)\, dV = \int_S d\mathbf{S} \cdot (\Gamma \nabla \phi) = \sum_f \Gamma_f \mathbf{S}_f \cdot (\nabla \phi)_f \tag{A.12}$$

The face gradient discretization is implicit when the length vector d between the center of the cell of interest P and the center of the neighboring cell N is orthogonal to the face plane, i.e., parallel to $\mathbf{S}_f$:

$$\mathbf{S}_f \cdot (\nabla \phi)_f = |S_f| \, \frac{\phi_N - \phi_P}{|d|} \tag{A.13}$$

In the case of non-orthogonal meshes, an additional explicit term is introduced which is evaluated by interpolating cell center gradients, themselves calculated by central differencing cell center values.

Source Terms

Source terms can be specified in three ways: explicit, implicit, and implicit/explicit. For explicit source terms, they are incorporated into an equation simply as a field of values. For example, to solve Poisson's equation $\nabla^2\phi = f$, ϕ and f would be defined as `volScalarField` and then do

```
solve(fvm::laplacian(phi) == f)
```

In contrast, an implicit source term is integrated over a control volume and linearized by

$$\int_V S_\phi(\phi)\, dV = SpV_P\phi_P$$

The Implicit/Explicit approach changes between the two based upon the sign of the source term. If the source is positive, it is treated as an implicit source term so that it increases the diagonal dominance of the matrix. If the source is negative, it is treated as an explicit source term. In mathematical terms, the mixed source approach can be written as

$$\int_V S_\phi\left(\phi\right)\, dV = SuV_P + SpV_P\phi_P \tag{A.14}$$

A.2.2 Temporal Discretization

Temporal Derivatives

The first derivative $\partial\partial t$ is integrated over a control volume with one of two schemes: 1st-order Euler implicit, or 2nd-order backward difference

$$\frac{\partial}{\partial t}\int_V \rho\phi\, dV = \frac{\left(\rho_P\phi_P V_P\right)^n - \left(\rho_P\phi_P V_P\right)^0}{\Delta t} \tag{A.15}$$

$$\frac{\partial}{\partial t}\int_V \rho\phi\, dV = \frac{3\left(\rho_P\phi_P V_P\right)^n - 4\left(\rho_P\phi_P V_P\right)^0 + \left(\rho_P\phi_P V_P\right)^{00}}{2\Delta t} \tag{A.16}$$

where the new values are $\phi^n = \phi(t+\Delta t)$, the old values are $\phi^0 = \phi(t)$, and the old-old values are $\phi^{00} = \phi(t-\Delta t)$.

Treatment of Spatial Derivatives in Transient Problems

Reconsider the integral form of the transport equation Eq. (A.5).

$$\int_t^{t+\Delta t}\left[\frac{\partial}{\partial t}\int_{V_p}\rho\phi\, dV + \int_{V_p}\nabla\cdot\left(\rho\mathbf{U}\phi\right)\, dV - \int_{V_p}\nabla\cdot\left(\rho\Gamma_\phi\nabla\phi\right)\, dV\right] dt = \int_t^{t+\Delta t}\left[\int_{V_p} S_\phi\left(\phi\right)\, dV\right] dt$$

Using Eqs. (A.7), (A.12), and (A.14), Eq. (A.5) can be written in a semi-discretized form

$$\int_t^{t+\Delta t}\left[\frac{\partial}{\partial t}\int_{V_p}\rho\phi\, dV + \sum_f F\phi_f - \sum_f\left(\rho\Gamma_\phi\right)\mathbf{S}\cdot\left(\nabla\phi\right)_f\right] dt = \int_t^{t+\Delta t}\left(SuV_P + SpV_P\phi_P\right)\, dt \tag{A.17}$$

For an Euler implicit approach, this equation can be reduced to

$$\frac{(\rho_P \phi_P V_P)^n - (\rho_P \phi_P V_P)^0}{\Delta t} + \sum_f F \phi_f^n - \sum_f (\rho \Gamma_\phi)\, \mathbf{S} \cdot (\nabla \phi)_f^n = (SuV_P + SpV_P \phi_P^n) \tag{A.18}$$

In contrast, Eq. (A.17) can also be evaluated with a Crank-Nicholson scheme. The result is

$$\frac{(\rho_P \phi_P V_P)^n - (\rho_P \phi_P V_P)^0}{\Delta t} + \sum_f F \left(\frac{\phi_f^n + \phi_f^0}{2} \right) - \sum_f (\rho \Gamma_\phi)\, \mathbf{S} \cdot \left(\frac{(\nabla \phi)_f^n + (\nabla \phi)_f^0}{2} \right) = SuV_P + SpV_P \left(\frac{\phi_P^n + \phi_P^0}{2} \right) \tag{A.19}$$

Regardless of the approach, the equations can be reduced to the algebraic system for every control volume

$$a_P \phi_P^n + \sum_N a_N \phi_N^n = R_P \tag{A.20}$$

where the coefficients a_P and a_N are the diagonal and off-diagonal coefficients, respectively, and R_P is the source-term vector.

A.3 Solution Algorithm for the Navier-Stokes Equations

Solution of the incompressible Navier-Stokes equations requires that three items be addressed: derivation of an equation for pressure; linearization of the momentum equations; and implementation of a pressure-velocity coupling algorithm. These items will be discussed in the following sections.

A.3.1 Linearization

The nonlinear convection terms in equations A.2 are reduced to $\sum_f F \phi_f^n$ where $F = \mathbf{S} \cdot (\mathbf{U})_f$. The challenge is that F, and a_P and a_N from Eq. (A.20), are functions of (U). The important issue is that the fluxes F should satisfy the continuity equation, equation A.1. Linearization of the convection term means that the existing velocity (or flux) field that satisfies continuity will be used to calculate a_P and a_N. For strongly nonlinear phenomenon, two approaches can be used to capture the nonlinearity: sub-iteration over the entire algorithm such that the lagged velocities, and therefore the fluxes and coefficients, are iteratively updated; or use of small time-s such that the error in not updating the fluxes and coefficients remains small. Both impose a computational cost.

A.3.2 Derivation of the Pressure Equation

A semi-discrete form of the momentum equations is used to derive the pressure equation:

$$a_P \mathbf{U}_P = \mathbf{H}(\mathbf{U}) - \nabla p \tag{A.21}$$

This equation is clearly an extension of Eq. (A.20), however, the pressure term has been broken out, and $\mathbf{H}(\mathbf{U})$ consists of two parts, the "transport part" which includes the matrix of coefficients for all neighbors multiplied by corresponding velocities, and the "source-term part" which includes part of the transient term and all other source terms (apart from the pressure gradient). For

example, $\mathbf{H}(\mathbf{U})$ for the incompressible NS equations (excluding source terms due to gravity and turbulence) using Euler implicit temporal differencing is

$$\mathbf{H}(\mathbf{U}) = -\sum_N a_N \mathbf{U}_N + \frac{\mathbf{U}^0}{\Delta t} \tag{A.22}$$

Equation (A.21 can also be solved for the velocity at the cell center by dividing by a_P

$$\mathbf{U}_P = \frac{\mathbf{H}(\mathbf{U})}{a_P} - \frac{1}{a_P}\nabla p \tag{A.23}$$

From this, the velocity at the cell face can be found through interpolation, i.e.,

$$\mathbf{U}_f = \left(\frac{\mathbf{H}(\mathbf{U})}{a_P}\right)_f - \left(\frac{1}{a_P}\right)_p (\nabla p)_f \tag{A.24}$$

To derive the pressure equation, the discrete incompressible continuity equation is written

$$\sum_f \mathbf{S} \cdot \mathbf{U}_f = 0 \tag{A.25}$$

and Eq. (A.24) is inserted,

$$\nabla \cdot \left(\frac{1}{a_P}\nabla p\right) = \sum_f \mathbf{S} \cdot \left(\frac{\mathbf{H}(\mathbf{U})}{a_p}\right)_f \tag{A.26}$$

The Laplacian operator on the left-hand side can be discretized using the method described in Section A.2.1, which results in the final form of the discretized incompressible Navier-Stokes equations

$$a_P \mathbf{U}_P = \mathbf{H}(\mathbf{U}) - \sum_f \mathbf{S}(p)_f \tag{A.27}$$

$$\sum_f \mathbf{S} \cdot \left[\left(\frac{1}{a_P}\right)_f (\nabla p)_f\right] = \sum_f \mathbf{S} \cdot \left(\frac{\mathbf{H}(\mathbf{U})}{a_P}\right)_f \tag{A.28}$$

Finally, if the face fluxes F are computed using U_f from Eq. (A.24),

$$F = \mathbf{S} \cdot \mathbf{U}_f = \mathbf{S} \cdot \left[\left(\frac{\mathbf{H}(\mathbf{U})}{a_P}\right)_f - \left(\frac{1}{a_P}\right)_p (\nabla p)_f\right] \tag{A.29}$$

then the fluxes are guaranteed to be conservative.

A.4 Pressure-Velocity Coupling

The discretized form of the Navier-Stokes system in Eqs. (A.27) and (A.28) are coupled in that each contains velocity and pressure. While there are algorithms for solving the fully-coupled set of equations, this remains computationally expensive in comparison to the segregated methods for coupling the pressure and velocity fields. The most common segregated methods are the PISO [17] and SIMPLE [18] algorithms and their derivatives (e.g., SIMPLE-C, SIMPLER). Both are commonly used in OpenFOAM, however, SIMPLE and PISO are typically used for steady and transient problems, respectively. Each is briefly discussed in the following sections.

The pressure-implicit split-operator (PISO) algorithm is a predictor-corrector approach for solving transient flow problems. For the PISO algorithm, the momentum equation is solved first, however, since the exact pressure gradient source term is not known at this stage, the pressure field from the previous time-step is used instead. This stage is called the momentum predictor and gives an approximation of the new velocity field. Using the predicted velocities, the $\mathbf{H}(\mathbf{U})$ operator can be assembled and the pressure equation can be formulated. The solution of the pressure equation gives the first estimate of the new pressure field. This step is called the pressure solution.

Next, conservative fluxes consistent with the new pressure field are computed using Eq. (A.29). The velocity field should also be corrected as a consequence of the new pressure distribution. Velocity correction is done in an explicit manner, using Eq. (A.23). This is the explicit velocity correction stage.

A closer look at Eq. (A.23) reveals that the velocity correction actually consists of two parts: a correction due to the change in the pressure gradient $\left(\frac{1}{a_P}\nabla p\right)$ and the transported influence of corrections of neighboring velocities $\left(\frac{\mathbf{H}(\mathbf{U})}{a_P}\right)$. The fact that the velocity correction is explicit means that the latter part is neglected. It is therefore necessary to correct the $\mathbf{H}(\mathbf{U})$ term, formulate the new pressure equation and repeat the procedure. In other words, the PISO loop consists of an implicit momentum predictor followed by a series of pressure solutions and explicit velocity corrections. The loop is repeated until a pre-determined tolerance is reached.

Another issue is the dependence of $\mathbf{H}(\mathbf{U})$ coefficients on the flux field. After each pressure solution, a new set of conservative fluxes is available. It would be therefore possible to recalculate the coefficients in $\mathbf{H}(\mathbf{U})$. This, however, is not done: it is assumed that the non-linear coupling is less important than the pressure-velocity coupling, consistent with the linearization of the momentum equation. The coefficients in $\mathbf{H}(\mathbf{U})$ are therefore kept constant through the whole correction sequence and will be changed only in the next momentum predictor.

The overall PISO algorithm can be summarized as follows:

1. Set the initial conditions.
2. Begin the time-marching loop.
3. Assemble and solve the momentum predictor equation with the available face fluxes (and pressure field).
4. Solve the pressure equation, and explicitly correct the velocity field. Iterate until the tolerance for pressure-velocity system is reached. At this stage, pressure and velocity fields for the current time-step are obtained, as well as the new set of conservative fluxes.
5. Using the conservative fluxes, solve all other equations in the system. If the flow is turbulent, calculate the eddy viscosity from the turbulence variables.
6. Go to the next time step, unless the final time has been reached.