DEPARTMENT OF CHEMICAL & PROCESS ENGINEERING

University of Strathclyde Engineering

ARCHIE-WeSt

Academic and Research Computer Hosting Industry and Enterprise in the West of Scotland

ANSYS Fluent CFD ARCHIE-WeSt HPC Manual

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Using this Manual:

Easily set-up large, memory intensive simulations in ANSYS Fluent

Dramatically reduce Fluent simulation time requirements

Quickly and effectively analyse simulation results and create animations

Write ANSYS Fluent HPC Job scripts

Gain experience with a HPC system

Effectively Transfer results to a local machine for storage and further analysis

Contents

1 Introduction

SimulationS of complex fluid systems requires the geometry to be divided into a large number of discrete elements which can be both computationally and memory extensive. High Performance Computing (HPC) systems such as ARCHIE-WeSt allow for the effective parallelisation of complex tasks, dramatically reducing the time between the construction of the geometry and the acquisition of results relative to serial desktop simulations. The computational ability of the ARCHIE-WeSt HPC system also provides the opportunity to simulate multiple systems at the same time with no loss of performance over a single HPC simulation. This opens the door to the effective optimisation of complex system geometry and process conditions. The ARCHIE-WeSt HPC system has the memory capacity and graphical ability to allow for the simulation and post-processing of highly detailed systems that would otherwise be impossible on some standard desktop computers. The current Fluent Licensing allows uses to run a single simulation on up to 32 computing cores.

1.1 What will this manual cover?

This manual will provide an in depth treatment of the following aspects:

- the basics of accessing, submitting jobs and transferring files to and from the ARCHIE-WeSt HPC system from both Windows and Linux local environments
- the various options available to set-up, simulate and post process ANSYS Fluent simulations using the ARCHIE-WeSt HPC system
- the set-up procedure of ANSYS Fluent simulations on the ARCHIE-WeSt HPC system
- the post processing options available to users using ANSYS CFD
- four comprehensive examples of large, computationally intensive systems relevant to chemical engineering processes simulated using ANSYS Fluent on the ARCHIE-WeSt HPC system (including example set-up scripts)
- an analysis of the performance increase available in ANSYS Fluent simulations on the ARCHIE-WeSt HPC system

1.2 Who is this manual aimed at?

This report is aimed at users who have intermediate to advanced knowledge of ANSYS CFD software (particularly ANSYS Fluent) who wish to significantly reduce the time required to perform and post-process ANSYS Fluent CFD simulations. This manual assumes that the user has a degree of familiarity with carrying out simple tasks on the Linux operating system; however, users who have had no experience of Linux are directed to the user section of the ARCHIE-WeSt HPC website (`http://www.archie-west.ac.uk`) for a comprehensive introduction to the basic Linux knowledge required to carried out simulations on the ARCHIE-WeSt HPC system It is assumed that the user already has a serial licensed version of ANSYS CFD (at least v14.0) installed on their local machine under Windows or a suitable Linux distribution.

1.3 Structure

We begin with an overview of the various options for accessing, submitting jobs and transferring data to and from the ARCHIE-WeSt HPC system. This is followed by a detailed walk-through of the pre-simulation files required (either on the user's local machine or the ARCHIE visualisation server) to perform a Fluent simulation and finally we detail the procedure for initiating a Fluent simulation as well as the post-processing options available to the user. The remainder of the manual is dedicated to four distinct worked examples of relevant chemical engineering problems which includes statistics on the meshes used, presentation of the actual scripts used to initiate and perform the simulation and finally a summary of the relative performance of the ARCHIE-WeSt HPC system.

1.4 Performance Metrics

To determine the scaling performance of Fluent simulations on the ARCHIE-WeSt HPC system, each example in this manual has been carried out on 4, 8 and 12 computational cores within ARCHIE. For the purposes of comparison, these simulations have also been carried out on a local desktop running Windows 7 Professional with a Dual Intel®Xeon®Processor E5-2620 v2 2.1GHz Turbo with 16GB 1866MHz RAM using a single core. Since each of the meshes used within this report are in excess of 500,000 elements in size, ANSYS licensing does not allow these cases to be simulated in serial mode on a local machine. Hence, each local simulation has been carried out in Fluent in Parallel mode, specifying a single core in the local case. Simulation performance is reported using the following normalisation:

$$\text{Speed} = \frac{\text{Wall clock simulation time with local single core Xeon®}}{\text{Wall clock simulation time on ARCHIE HPC}}$$

1.5 Disclaimer

This Fluent examples presented in this manual are for demonstration purposes only. No guarantees regarding the accuracy or correctness of the results obtained/methods used are made. All simulations carried out in this manual were performed using ANSYS Fluent v15.0. Commands and performance may differ slightly between versions.

2 Performing Fluent Simulations on ARCHIE-WeSt HPC

2.1 Accessing ARCHIE-WeSt HPC

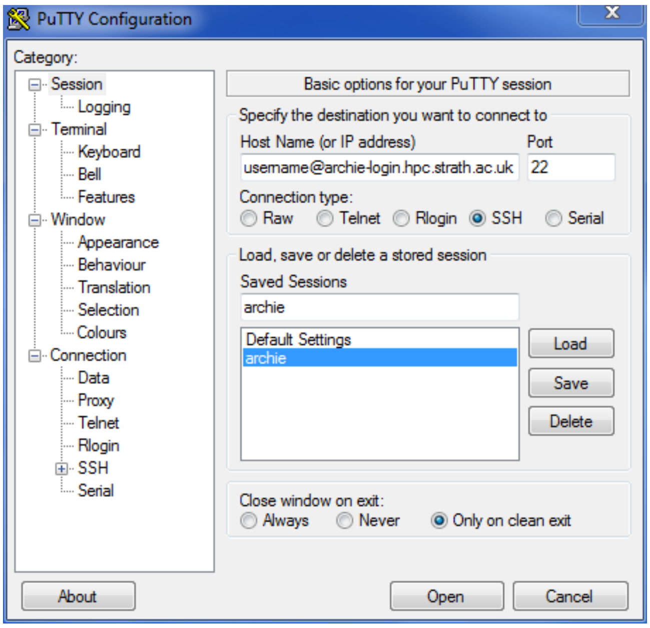
This section will give a brief overview of the log-in process from Windows and Linux environments and how files can be transferred between ARCHIE and the user's local machine. Detailed instructions on logging in and submitting generic jobs scripts to ARCHIE from both Windows and Linux environments can be found within the Training Materials at `http://www.archie-west.ac.uk` (log-in required).

2.1.1 Terminal only access from a Windows Environment

Logging in

If terminal only access to ARCHIE is required then it is recommended that users access ARCHIE using Putty. Putty is a free, easy to use 3rd party ssh client that can be downloaded from `http://www.chiark.greenend.org.uk/~sgtatham/putty/download.html`. Download and run *putty.exe* to start Putty.

When running Putty users will be required to log in with their DS username and password in the following format:



Once the user is successfully logged in to ARCHIE through Putty they will be presented with a Linux terminal from which they can navigate to the desired directories, submit jobs to the process queue etc.

2.1.2 GUI access from a Windows Environment

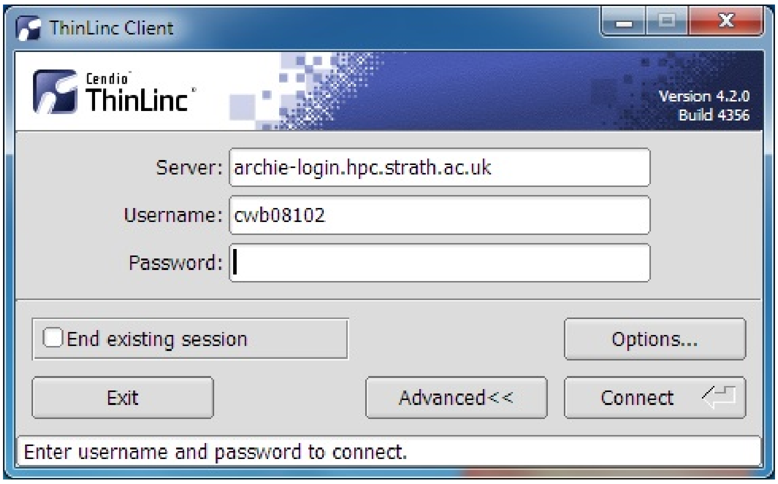
Logging in

A GUI interface to ARCHIE can be obtained using a Remote Desktop software package called ThinLinc which is produced by Cendio. This can be downloaded from `https://www.cendio.com/thinlinc/download`.

Once Downloaded, run the installer and install using the default options. To login to ARCHIE, start the ThinLinc client from the Programs menu and supply the server address:

```
archie-login.hpc.strath.ac.uk
```

Click on the "Advanced" and then the "Options" button to change the default options - the most useful of which is to select "Work Area (maximed)" from under the "Screen" tab. Supply your DS username and password to log in.



2.1.3 Uploading files to ARCHIE from a Windows Environment

It is recommended that any data required by Fluent such as case, data and journal files be uploaded to the users home directory on ARCHIE using WinSCP. WinSCP is a free and easy to use third party program that can be downloaded from `http://winscp.net/eng/download.php` (click Installation package to begin download).

Again, WinSCP will require the user to log-in with their DS username and password. The host server should be set to `archie-login.hpc.strath.ac.uk` and the port set to `22`. Once connected the user will be able to drag files to and from their local machine and their ARCHIE directories.

2.1.4 Accessing from Linux Environment

Logging in
ARCHIE can be easily accessed using the ssh protocol which requires your DS username and password. The following command should be entered within terminal window on the users local machine:

```
ssh USERNAME@archie-login.hpc.strath.ac.uk -X
```

Note: the `'-X'` *argument allows for the use of some GUIs within ARCHIE such as text editors (vi, emacs and gedit (gedit recommended)).*

You will be prompted for a password. Once you are successfully logged in the following message should be displayed:

```
USER@localhost:~/$ ssh USERNAME@archie-login.hpc.strath.ac.uk -X
USERNAME@archie-login.hpc.strath.ac.uk's password:
Last login: Mon Aug 18 16:47:30 2014 from user.pc.address

              +++++++++++++++++++++++++++++++++++++++++++++
                        Welcome to ARCHIE-WeSt
                      Based on Scientific Linux 6
              +++++++++++++++++++++++++++++++++++++++++++++

TIPS:

'module avail'            - show available application environments
'module add <modulename>' - add a module to your current environment

'qstat'                   - show summary of running jobs

==================================================================================
Project Summary for USERNAME (based on jobs completed by 3.00 am)
==================================================================================

Project         Core Hours (my contribution)    Core Hours (all users)  Allocation
-------         ----------------------------    ----------------------  ----------

=========
Disk Use
=========

Filesystem      used    quota   grace
----------      ----    -----   -----
/lustre         164.6G  800.0G
/users          2.1G    52.4G
```

Uploading files to ARCHIE

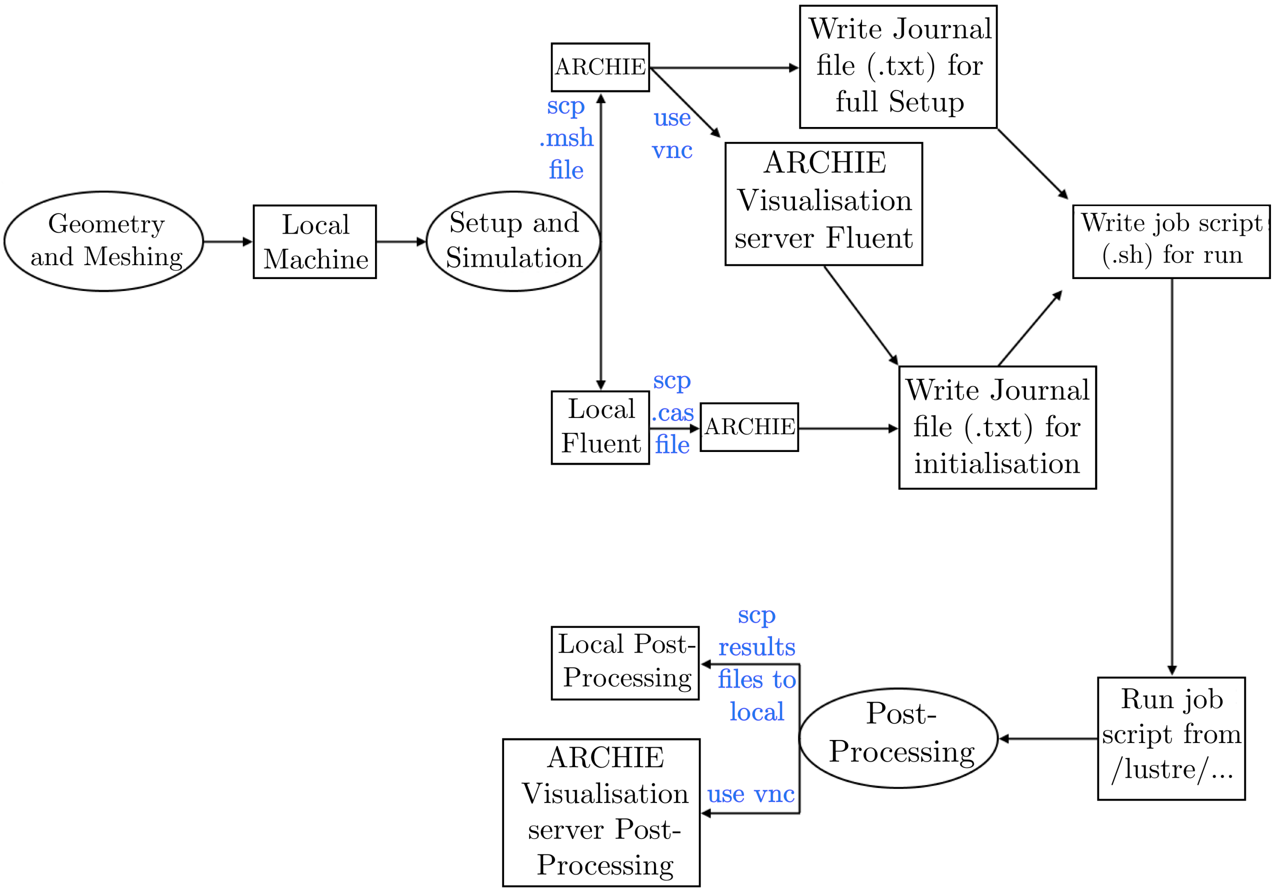
Data required by Fluent such as case, data and journal files should be uploaded to the users home directory on ARCHIE using the scp protocol on a terminal (Linux).

Example:

```
scp LOCAL_FILE_PATH USERNAME@archie-login.hpc.strath.ac.uk:
```

2.2 Work Flow Options

There are many routes the user may take to set-up, perform and post-process a Fluent simulation with the ARCHIE-WeSt HPC system. The route taken will generally be dictated by the size of the system to be simulated, the RAM capacity on the user's local machine and the user's post-processing requirements. The flow chart below is designed to help the user decide which route is best suited to their needs. The remainder of this section will walk the user through each of the steps outlined in the flow chart including instructions on acquiring/using any third party software required for specific steps.



2.3 Fluent Set-up

Meshing and Geometry related set-up are generally not RAM/CPU intensive tasks and should therefore be carried out on the user's local machine. As seen from the flowchart above it is possible to set-up a Fluent simulation from the user's local machine; through the ARCHIE visualisation nodes and directly through TUI commands within command line ANSYS on ARCHIE. This section will give an overview of the set-up process on ARCHIE (command line and visualisation nodes).

2.3.1 Set-up via the ARCHIE visualisation nodes

RAM intensive jobs may exceed the memory requirements of some older machines or machines which are required to perform several tasks in parallel. In such cases the set-up can be carried out on the ARCHIE system using a graphical version of Fluent on the dedicated visualisation nodes. In such cases the user would first upload the relavent mesh file on to the ARCHIE system. Note that simulations should not be carried out directly on these nodes ajnd should still be submitted to the queue.

Accessing the ARCHIE visualisation servers

Fluent can be run graphically within a "remote desktop" environment using the ThinLinc software as described in section 2.1.2. However, in this case, the server address that should be used is:

```
archie-viz.hpc.strath.ac.uk
```

The visualization servers have high-end graphics cards installed which allow graphical applications to be displayed efficiently across the network. When launching an application e.g Fluent, the command must be prefixed by **vglrun** to force it to use the on-board graphics card i.e.

```
vglrun fluent 3d -ssh
```

Opening Fluent/CFD Post

Once the user has successfully logged in to the remote desktop, Fluent can be opened via the terminal. A terminal window can be opened by clicking on the terminal icon in the task bar. To open Fluent from the terminal enter the following commands:

```
module load apps/bin/fluent/15.0.1
vglrun fluent 3d -ssh
```

The user may now load case/data files and set-up a Fluent simulation as would normally be done on a local machine. Note that the simulation should not be initialised or run at this point. These final steps (including patching and animation set-up) will be done through TUI commands within a journal file as described in Section 2.3.2.

To run CFD Post on the visualisation server enter the following commands:

```
module load apps/bin/ansys/15.0.1
vglrun cfdpost
```

2.3.2 Set-up via ANSYS TUI commands on ARCHIE

It is possible to completely define/run a Fluent simulation set-up using the Text User Interface (TUI) within the Fluent software. This involves reading commands from a journal file in specific sequence such that the desired set-up is achieved. However, this method can be prone to error. For example, the journal sequence may be correct in the case where an output file is not being overwritten, however; should an output file of the same name exists in the run directory then the TUI may ask additional questions regarding the overwrite. These will then be answered by next command in the sequence, generally resulting in an invalid answer and the journal inputs will no longer correspond to there intended questions. It is for this reason that we recommend that users unfamiliar with command line Fluent perform most of the simulation set-up through the Fluent Graphical User Interface (GUI) on their local machine and only carry out simple tasks such as initialising, patching and animation set-up via the TUI within the Fluent HPC Environment.

Set-ups and TUI commands should be tested on the users local machine to ensure the simulation is defined appropriately and allow for an estimation of the time required for the full simulation to be made (based on the time taken to carry out a small number of iterations).

After setting up the simulation on a local version of Fluent the user should export the case file (and data if required) to their local machine for transfer to the ARCHIE system.

An example of a Fluent script composed on TUI commands is given in Section 2.4.2 and further examples are contained within each of the Fluent cases presented within this manual.

2.4 Running a Fluent Simulation

ARCHIE jobs should be submitted from `/lustre/users-directory-path` where the users directory path is dependent on the project being carried out. All files required for a desired simulation to run should be copied to this directory prior to submitting the job.

A Fluent simulation job on ARCHIE will require at least three input files: a Fluent case file (.cas or .cas.gz); a shell script (.sh) and a Fluent journal file (generally .jou or .txt).

2.4.1 The Job Script

The job script (.sh) will carry out the following:

- load the modules required to run Fluent
- define how many computing cores will be used for the simulation
- define which ARCHIE computational nodes will be used
- identify the project with which the job is associated
- provided an estimation of the total simulation time
- define the Fluent journal file to be read in
- define the number of dimensions/precision of the simulation
- initiate Fluent

An example shell script is presented below. Template job scripts can also be downloaded from the users section of the ARCHIE-WeSt website (`http://www.archie-west.ac.uk`). Examples can also be found within the job-scripts directory under the user's home directory on ARCHIE. This script should be saved in the lustre directory in which the simulation will be carried out.

```
#!/bin/bash

module load apps/bin/fluent/15.0.1

# ************* SGE qsub options ****************
#Export env variables and keep current working directory
#$ -V -cwd
#Select parallel environment and number of parallel queue slots (cores)
#$ -pe multiway 4
#Defining the project name
#$ -P PROJECTNAME.prj
#Combine STDOUT/STDERR
#$ -j y
#Specify output file
#$ -o out.$JOB_ID.doc
```

```
#Request resource reservation (reserve slots on each scheduler
#run until enough have been gathered to run the job
#$ -R y
# Add runtime indication
#$ -ac runtime="11hr"
# ************** END SGE qsub options ************

#Initiating Fluent and reading .txt file
fluent 3d -pib -ssh -sge -g -i example_1_fluent_input.txt output
```

IMPORTANT: To initiate Fluent in Double Precision mode `3d` would be replaced with `3ddp`.

To submit a job script simply enter the following command:

```
qsub JOB_SCRIPT_NAME.sh
```

The output of the TUI (showing residuals of simulation parameter etc) are sent to `out.JOBID` in the directory from which the job was submitted. The status of this job can be checked by entering `qstat` within the ARCHIE terminal.

For more information on running, checking and cancelling jobs please see the training materials within the users section of the ARCHIE website (`http://www.archie-west.ac.uk`).

Output data can be downloaded from ARCHIE to the users local machine again using the Putty (local Windows environment). Linux users can use the scp protocol from ARCHIE as shown below:

```
scp OUTPUT_FILE LOCAL_USERNAME@LOCAL_IP:DESTINATION_PATH
```

Alternatively, Linux users can carry out the scp command from their local machine using:

```
scp USERNAME@archie-login.hpc.strath.ac.uk:OUTPUT_FILE_PATH DESTINATION_PATH
```

2.4.2 Fluent Input Script

As mentioned previously the journal file required to start a Fluent simulation will be composed of TUI commands. A comprehensive list of the ANSYS Fluent TUI commands can be found within the ANSYS Customer Portal at `http://www.ansys.com/en_uk`. An example journal file (including additional comments) is given below.

```
;Example 1 Full Shell and Tube Heat Exchanger Unsteady Flow Field
;
;Reading in the case file
rc full_sthe.cas.gz
;
;hybrid initialising the system
solve/init/hyb-init
;
;Setting the transient time step size
solve/set/time-step 0.01
```

```
;
;Setting the number of time-steps (first number) and the max
;number of iterations per step (second number)
solve/dual-time-iterate 1000 1000
;
;Outputting solver performance data upon completion of the simulation
parallel timer usage
;
;Writing the final case file (overwriting if required)
wc full_sthe_out.cas.gz
yes
;
;Writing the final data file (overwriting if required)
wd full_sthe_out.dat.gz
yes
;Exiting Fluent
exit
yes
```

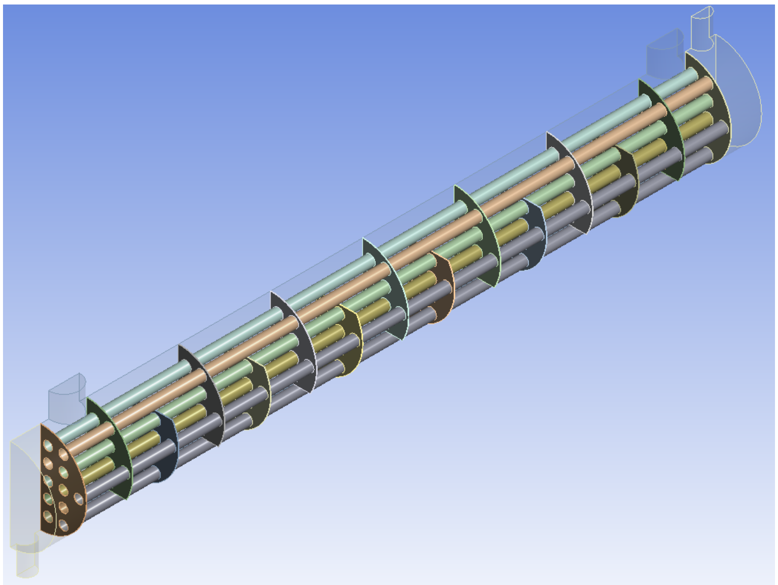
A Note on Animations

As described previously, the output of simulation can be processed both on the user's local machine and on the ARCHIE visualisation nodes. This will allow for the analysis of the solution to a steady state simulation of the final state of a transient simulation. However, since ARCHIE runs a non graphical version of ANSYS Fluent (v14 and v15) it is not possible to directly generate plots during the simulation (such as thermal contours plots at each time-step of a transient simulation). To analysis transient data at various points in the simulation history the user must specify the frequency at which data files (.cdat files) should be output in the Fluent set-up. The user must also specify which data should be output to such files for analysis. These files can then be read into CFD Post as a single case history and used to view the evolution of the system and generate animations. Users with limited to no experience of this method are directed to Appendix 9 which includes a detailed walk-though of the process.

3 Full Shell and Tube Heat Exchanger Unsteady Flow Field Example

3.1 Problem Statement

This example will consider a simplistic water-water shell and tube heat exchanger with a single shell pass (both fluids), 22 tubes, 13 baffles and rounded shell-side end-plates operating in counter-flow. In order to reduce computation time this example will only analyse the flow field through the exchanger and will not consider thermal flows within the system. Full-thermal treatment of a simplified analogue of this system is presented in Section 4 of this manual. The geometry of the full exchanger is shown below.



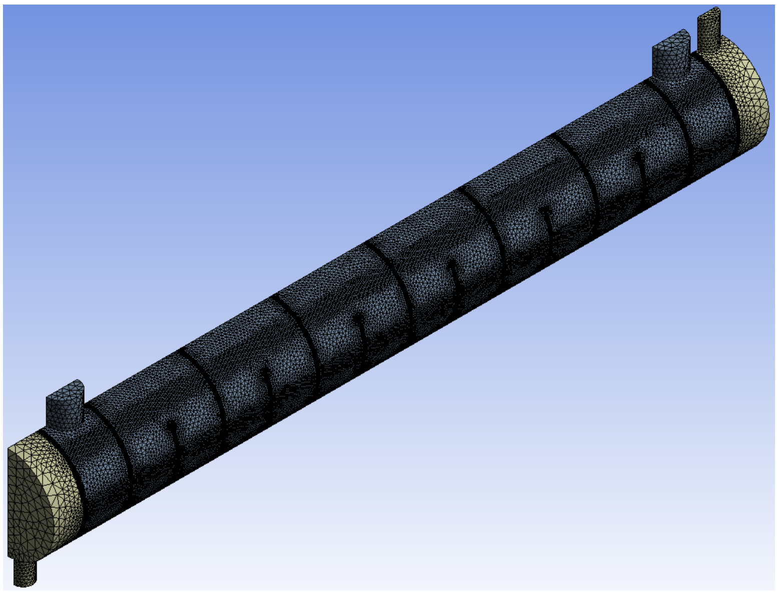
This geometry file can be found on ARCHIE at /opt/gridware/examples/fluent. The process conditions are summarised in Table 1.

Table 1: Summary of process conditions

Region	Fluid	Inlet velocity/[m.s^{-1}]	Boundary material	Flow regime
shell side	water	0.1	copper	Turbulent
tube side	water	0.1	copper	Turbulent

Due to the presence of baffles and high velocity flow within the exchanger it is likely that vortex shedding will be present within the shell side fluid. To account for the inherent unsteady nature of the system it will be simulated using the Fluent transient solver.

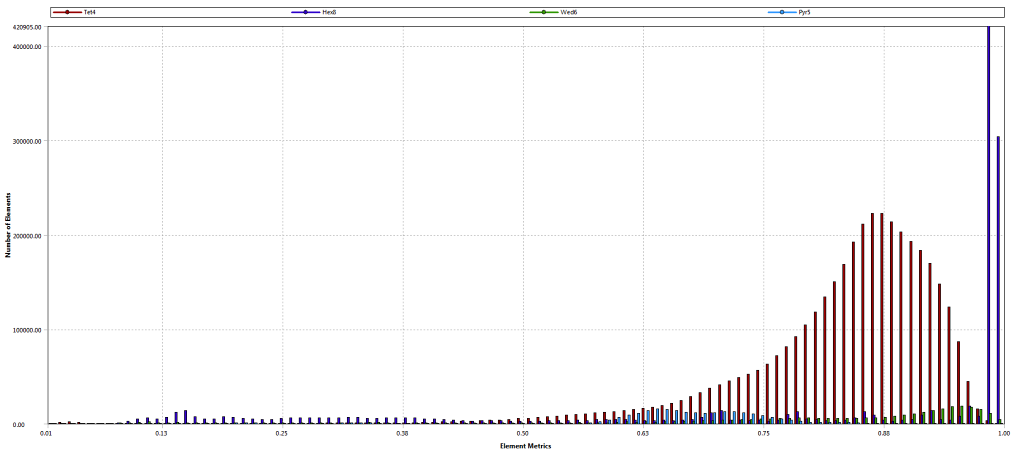
3.2 Details of The Mesh



Due to the complex nature of this design the number of elements required for effective simulation of the system is particularly large. The details of the resulting mesh are detailed in Table 2.

Table 2: Details of the mesh

Nodes	2096892
Elements	5539546
Mesh Metric	Orthogonal Quality
Min	5.050512E-03
Max	0.999637
Average	0.820966
Standard Dev.	0.167196
Approximate RAM usage	1.0GB



This mesh file can be found on ARCHIE in /opt/gridware/examples/fluent.

3.3 Details of the Local Fluent Set-up

The details of the Fluent set-up defined on the local machine prior to uploading to the ARCHIE system are defined within the .cas file which can be found in /opt/gridware/examples/fluent.

3.4 ARCHIE Scripts

3.4.1 The Job Script

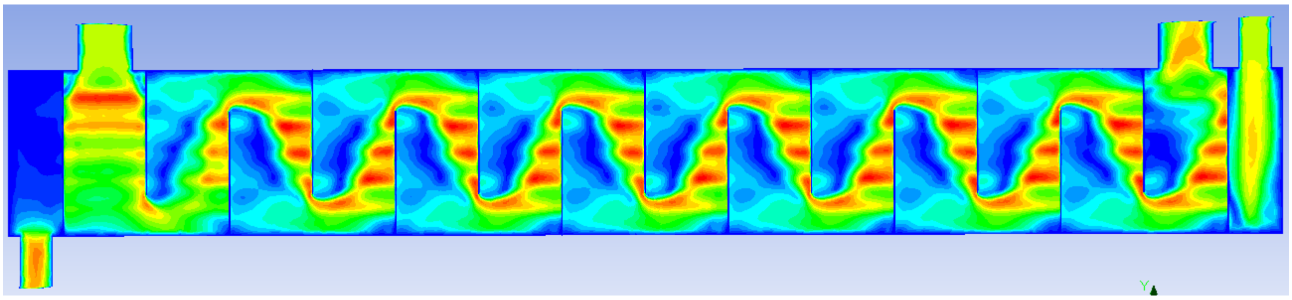
Please see Section 2.4.1.

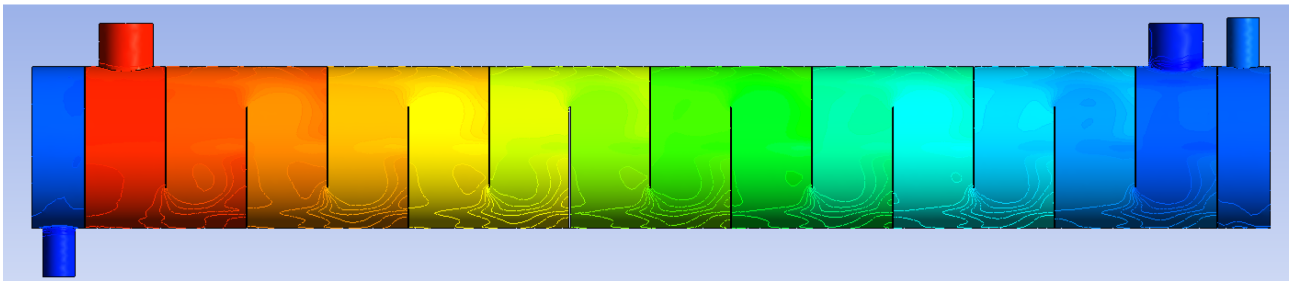
3.4.2 Fluent Input Script

Please see Section 2.4.2.

3.5 Results

The following velocity and pressure profiles were generated on a local machine within CFD Post from ARCHIE Fluent simulation data. Animations generated from this simulation can also be found on the ARCHIE web-page.



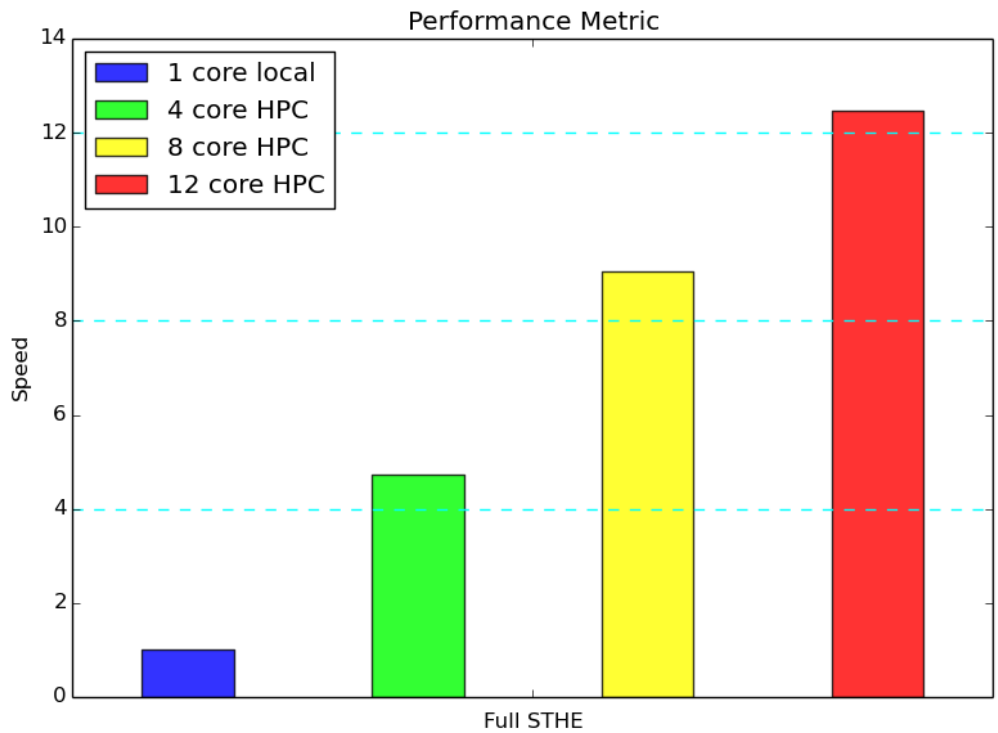


3.6 Performance

The computational performance of each simulation carried out is detailed in Table 3 and the relative performance illustrated below.

Table 3: Summary of performance over selected number of computing cores (ARCHIE HPC and local machine)

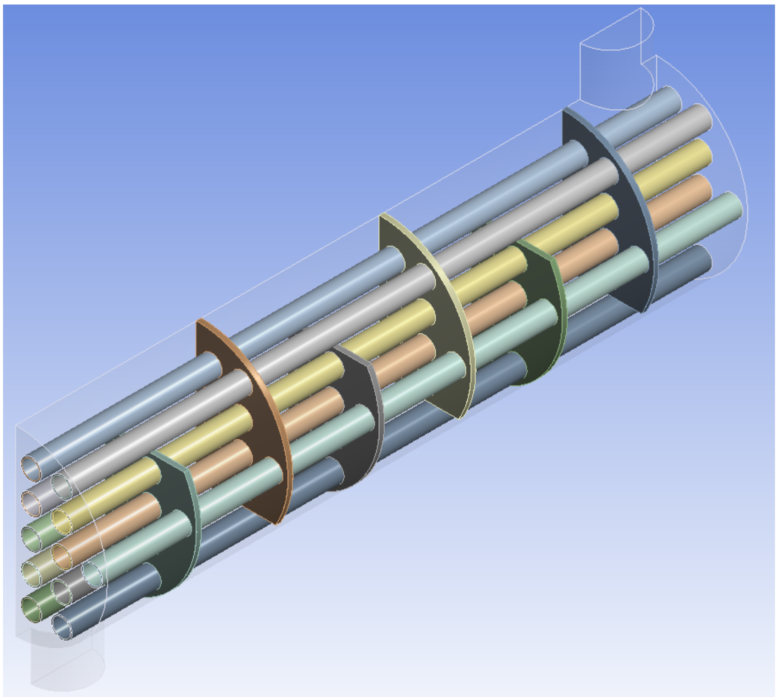
Number of Cores (System)	1 (Local)	4 (ARCHIE)	8 (ARCHIE)	12 (ARCHIE)
Simulation Wall-Clock Time (hours)	51.2	10.8	5.7	4.1
Total CPU Time (hours)	51.2	44.0	45.6	49.1



4 Partial Shell and Tube Heat Exchanger Thermal Analysis Example

4.1 Problem Statement

This example will consider the full thermal treatment of a partial shell and tube heat exchanger system operating in counter-flow as shown below. The geometry consists of 6 baffles, 11 tubes and complete shell side flow with inlet and outlet. The inlet/outlet of the tube side fluid are not fully modelled in order to reduce the computational time of case.



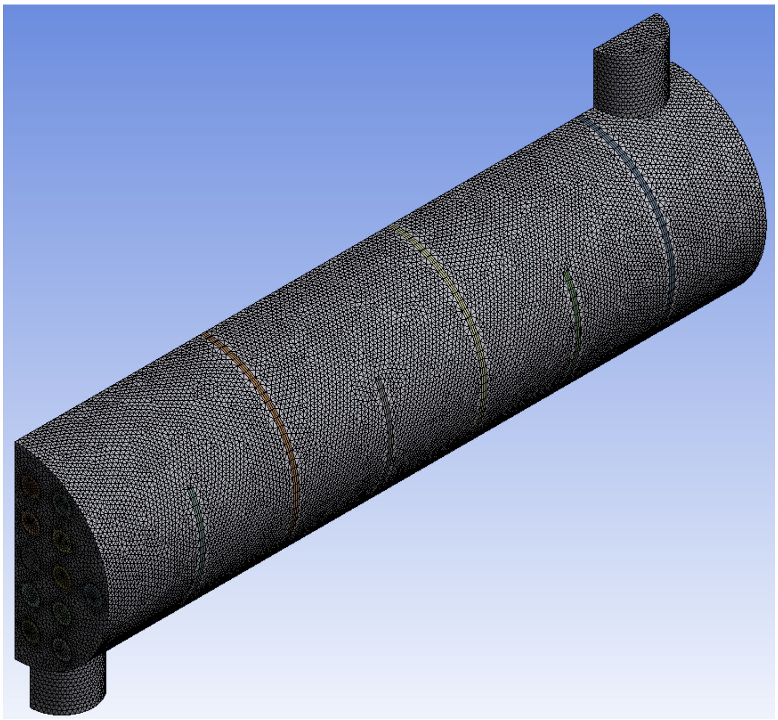
This geometry file can be found on ARCHIE at /opt/gridware/examples/fluent. The process conditions are summarised in Table 4.

Table 4: Summary of process conditions

Region	Fluid	Inlet velocity/[$m.s^{-1}$]	T/[K]	Boundary material	Flow regime
shell side	water	1.0	288.15	copper	Turbulent
tube side	water	1.0	363.15	copper	Turbulent

Due to the presence of baffles and high velocity flow within the exchanger it is likely that vortex shedding will be present within the shell side fluid. To account for the inherent unsteady nature of the system this system will be simulated using the Fluent transient solver.

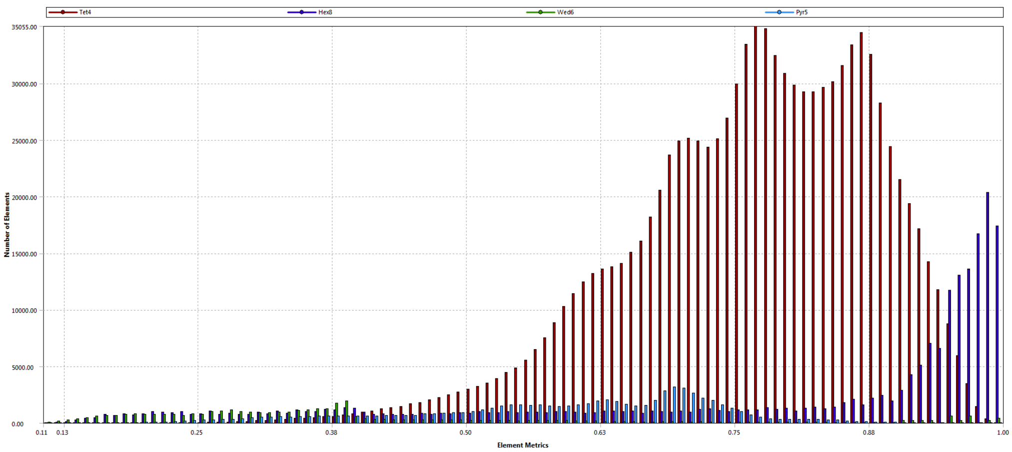
4.2 Details of The Mesh



Due to the complex nature of this design the number of elements required for effective simulation of the system is particularly large. The details of the resulting mesh are detailed in Table 5.

Table 5: Details of the mesh

Nodes	438591
Elements	1355455
Mesh Metric	Orthogonal Quality
Min	0.10568
Max	0.99999
Average	0.75183
Standard Dev.	0.16398
Approximate RAM usage	0.6GB



The mesh file can be found on ARCHIE at /opt/gridware/examples/fluent.

4.3 Details of the Local Fluent Set-up

The details of the Fluent set-up defined on the local machine prior to uploading to the ARCHIE system. For details of this set-up please see the .cas file which can be found on ARCHIE at /opt/gridware/examples/fluent.

4.4 ARCHIE Scripts

4.4.1 The Job Script

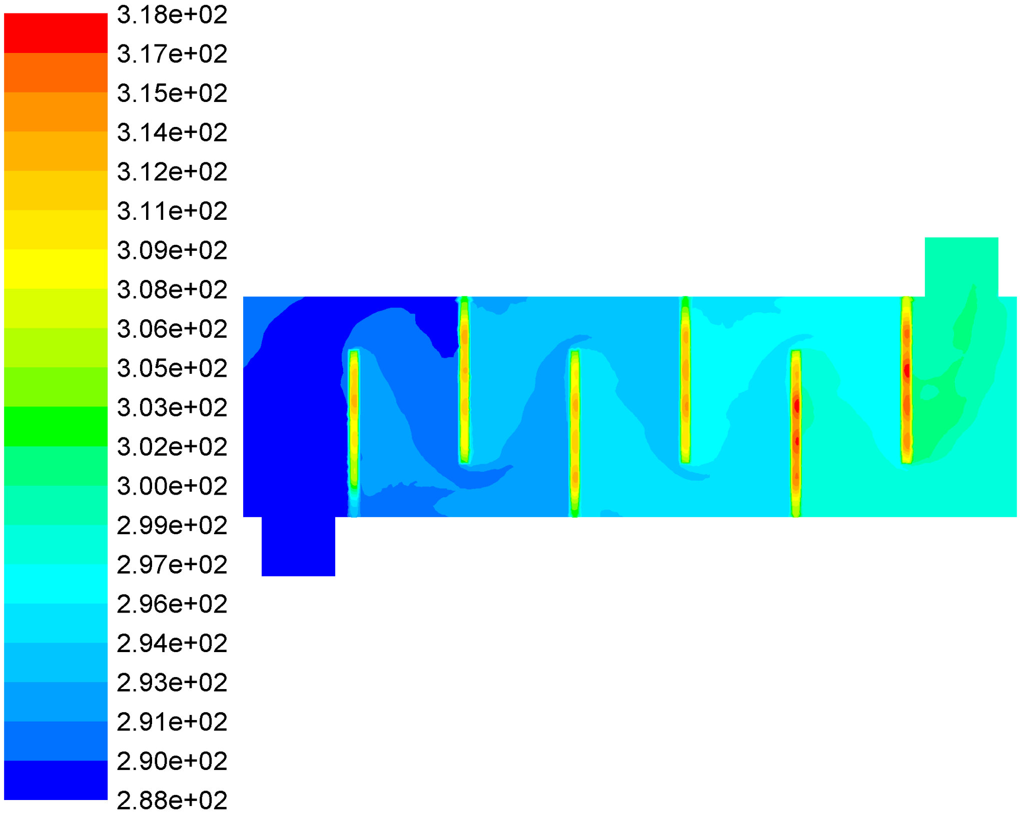
```
#!/bin/bash

module load apps/bin/fluent/15.0.1

# ************* SGE qsub options ***************
#Export env variables and keep current working directory
#$ -V -cwd
#Select parallel environment and number of parallel queue slots (cores)
#$ -pe multiway 4
#$ -P PROJECTNAME.prj
#Combine STDOUT/STDERR
#$ -j y
#Specify output file
#$ -o out.$JOB_ID
#Request resource reservation (reserve slots on each scheduler run
#until enough have been gathered to run the job
#$ -R y
# Add runtime indication
#$ -ac runtime="19h"
# ************** END SGE qsub options ************

#Initiating Fluent and reading .txt file
fluent 3ddp -pib -ssh -sge -g -i example_2_fluent_input.txt > output
```

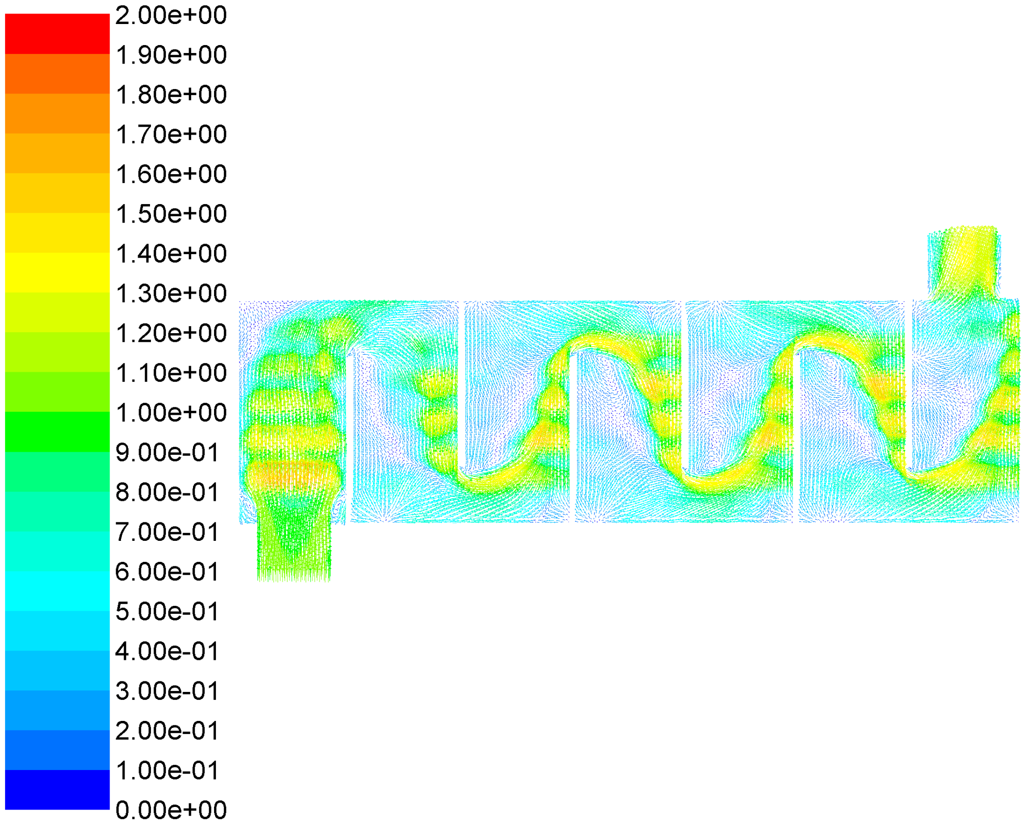
4.4.2 Fluent Input Script

```
;Example 2:  Partial Shell and Tube Heat Exchanger Thermal Analysis
;
;Reading in the case file
rc part_sthe.cas.gz
;
;Standard initialisation
solve/init/init
;
;Setting the solver time step (sec)
solve/set/time-step 0.01
;
;Setting the number of transient time-steps (first number) and the
;max no.  of iterations per time-steps
solve/dual-time-iterate 2000 1000
;
;Reporting the solver performance once the simulation has finished
parallel timer usage
;
;Writing the new case file (over-writing if necessary)
wc part_sthe_out.cas.gz
yes
;
;Writing the data file (over-writing if necessary)
wd part_sthe_out.dat.gz
yes
;
;Exiting Fluent
exit
yes
```

4.5 Results

The following thermal map and velocity vector field were generated on a local machine within CFD Post using the ARCHIE Fluent simulation data. Animations generated from these simulations can be found on the ARCHIE-WeSt web-page.



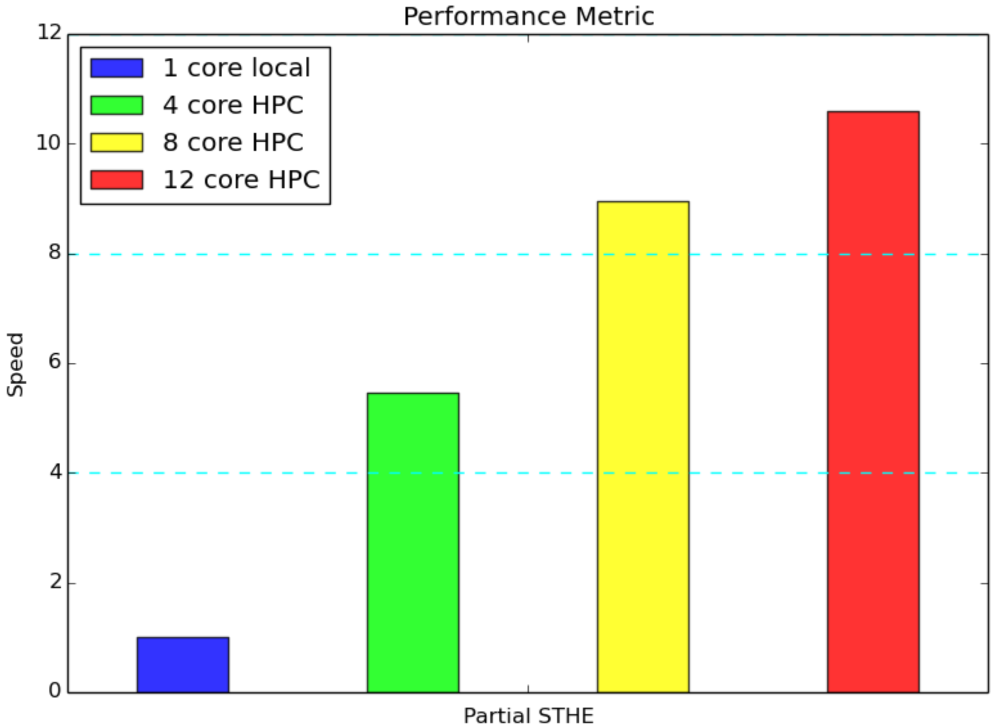


4.6 Performance

The computational performance of each simulation carried out is detailed in Table 6 and the relative performance below.

Table 6: Summary of performance over selected number of computing cores (ARCHIE HPC and local machine)

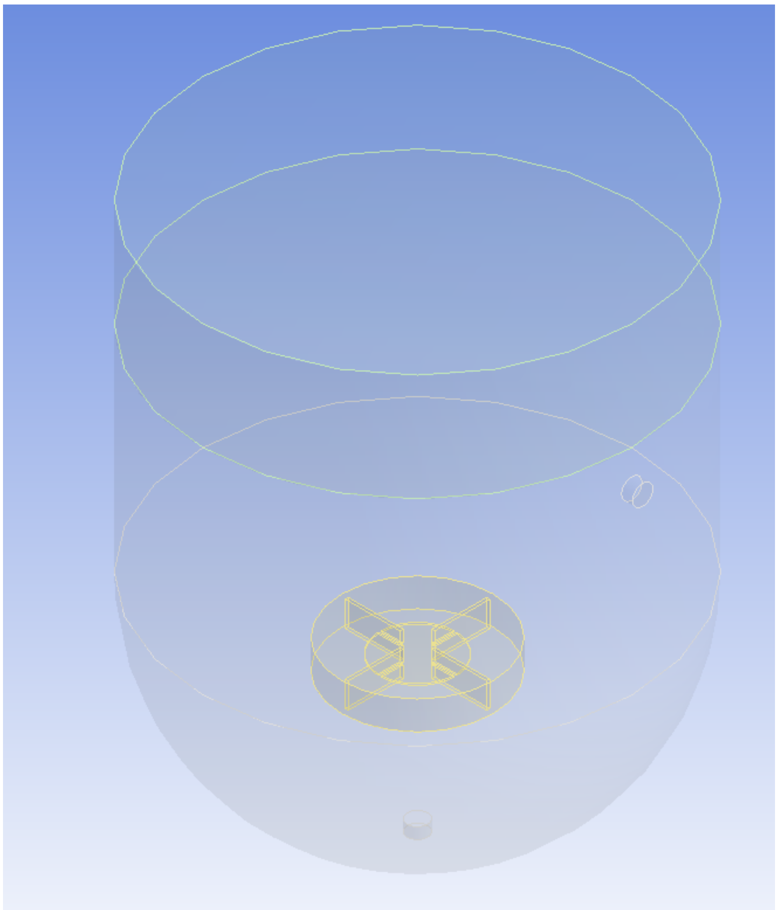
Number of Cores (System)	1 (Local)	4 (ARCHIE)	8 (ARCHIE)	12 (ARCHIE)
Simulation Wall-Clock Time (hours)	53.5	9.8	6.0	5.0
Total CPU Time (hours)	53.5	39.7	48.2	60.4



5 Air-Water Mixing Vessel Example

5.1 Problem Statement

In this example we consider a continuous multiphase system in which pure liquid water enters and leaves an agitated vessel with an air filled head space. The agitation is carried out by a simple rushton turbine. For simplicity of meshing and set-up the axle of the agitator is not modelled and the vessel is unbaffled. The geometry of the vessel is shown below.



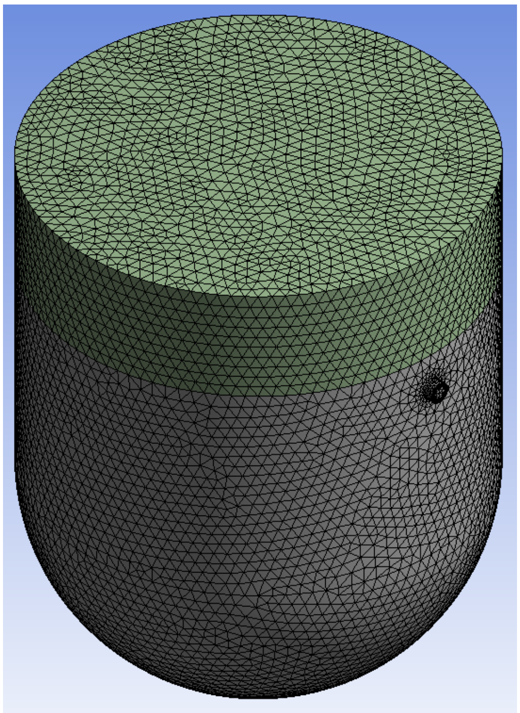
This geometry file can be found on ARCHIE at /opt/gridware/examples/fluent. The processing conditions are summarised in Table 7.

Table 7: Summary of process conditions

Vessel Volume /[m^3]	Liquid Volume /[m^3]	Agitator Type	Agitator Speed /[rmp]	Inlet Velocity /[$m.s^{-1}$]
18.29	14.63	Rushton turbine	100	0.4

Due to the presence of the agitator within the vessel it is likely that vortex shedding will be present around impeller blades. To account for the inherent unsteady nature of the system this system will be simulated using the Fluent transient solver.

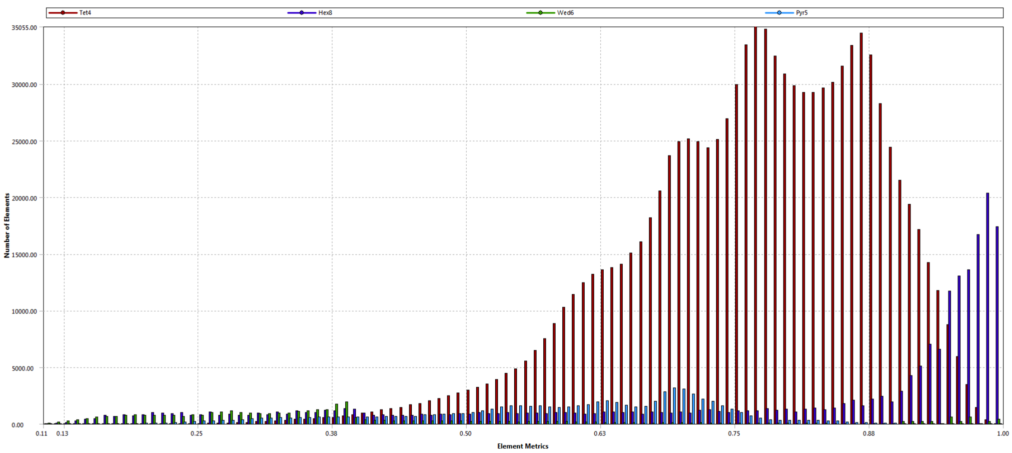
5.2 Details of The Mesh



Due to the complex nature of this design the number of elements required for effective simulation of the system is particularly large . The details of the resulting mesh are detailed in Table 8.

Table 8: Details of the mesh

Nodes	265386
Elements	1253380
Mesh Metric	Orthogonal Quality
Min	0.26131
Max	0.99994
Average	0.82824
Standard Dev.	0.10116
Approximate RAM usage	0.8GB



The mesh file can be downloaded found on ARCHIE at /opt/gridware/examples/fluent.

5.3 Details of the Local Fluent Set-up

The details of the Fluent set-up defined on the local machine prior to uploading to the ARCHIE system. For details of this set-up please see the .cas file available at /opt/gridware/examples/fluent.

5.4 ARCHIE Scripts

5.4.1 The Job Script

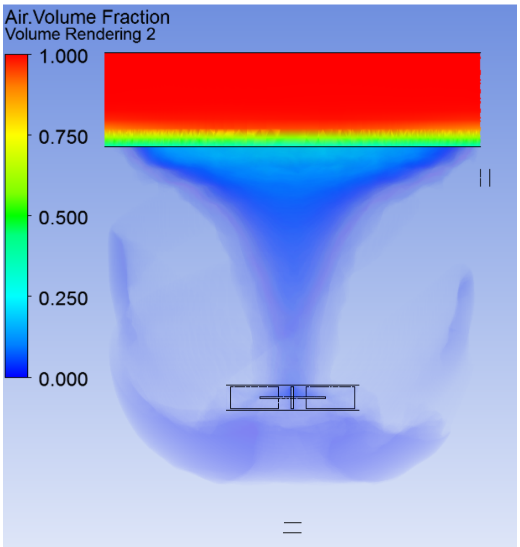
```
#!/bin/bash

module load apps/bin/fluent/15.0.1

# ************* SGE qsub options ****************
#Export env variables and keep current working directory
#$ -V -cwd
#Select parallel environment and number of parallel queue slots (nodes)
#$ -pe multiway 4
#$ -P PROJECTNAME.prj
#Combine STDOUT/STDERR
#$ -j y
#Specify output file
#$ -o out.$JOB_ID
#Request resource reservation (reserve slots on each scheduler run until
enough have been gathered to run the job
#$ -R y
# Add runtime indication
#$ -ac runtime="5h"
# ************** END SGE qsub options ************

#Initiating Fluent and reading .txt file
fluent 3d -pib -ssh -sge -g -i example_3_fluent_input.txt > output
```

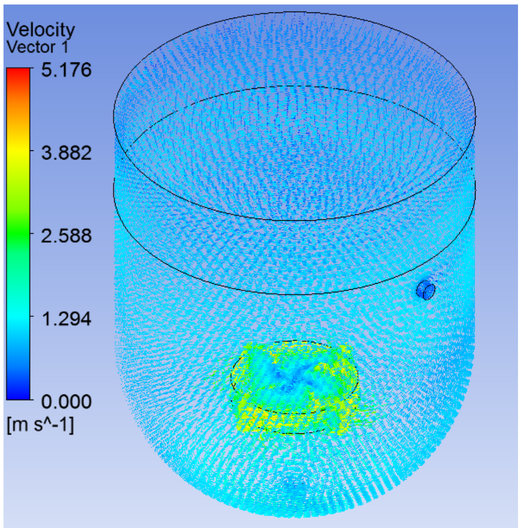
5.4.2 Fluent Input Script

```
;Example 3:  Air Water Mixing Vessel
;
;Reading in the case file
rc cstr_water_air_nb_tran.cas.gz
;
;Hybrid initialising the simulation
solve/init/hyb-init
;
;Patching the head space with air
solve patch air air

mp 1
;
;Setting the time-step size (sec)
solve set time-step 0.01
;
;Setting the number of time-steps (first number) and max
;number of iterations per time-step (second number)
solve/dual-time-iterate 5000 1000
;
;Reporting the performance after the simulation has finished
parallel timer usage
;
;Writing the new case file (over-writing if necessary)
wc cstr_wa_nb_tran_out.cas.gz
yes
;
;Writing the data file (over-writing if necessary)
wd cstr_wa_nb_tran_out.dat.gz
yes
;Exiting Fluent
exit
yes
```

5.5 Results

The following images were generated on a local machine within CFD Post using the ARCHIE Fluent simulation data.



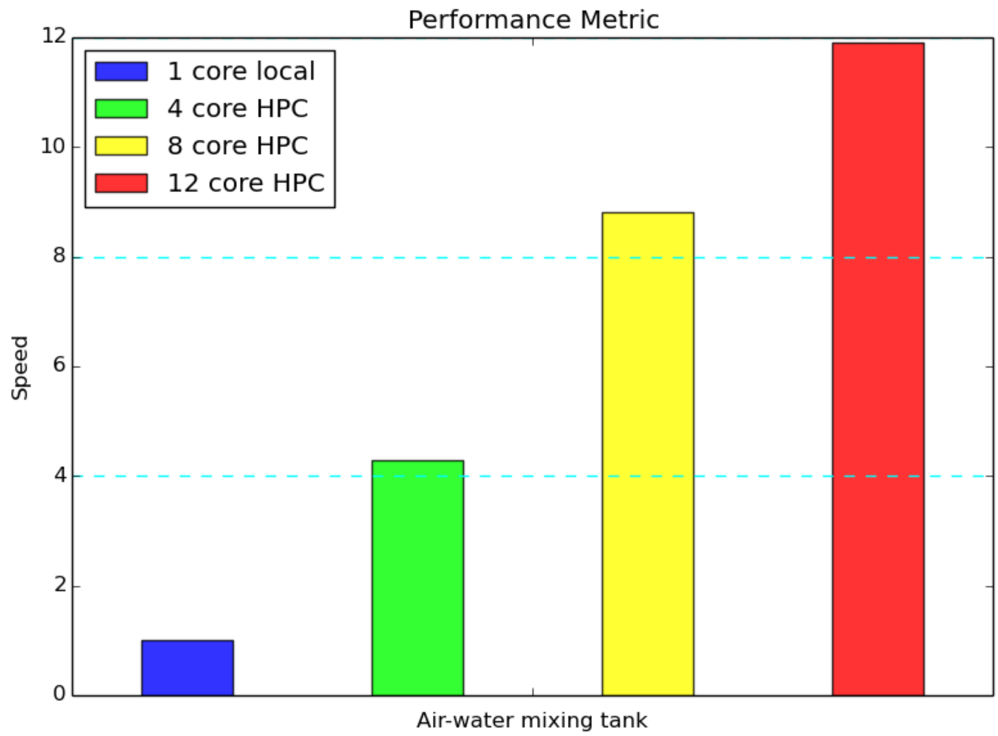


5.6 Performance

The computational performance of each simulation is detailed in Table 9 and the relative performance illustrated below.

Table 9: Summary of performance over selected number of computing cores (ARCHIE HPC and local machine)

Number of Cores (System)	1 (Local)	4 (ARCHIE)	8 (ARCHIE)	12 (ARCHIE)
Simulation Wall-Clock Time (hours)	20.6	4.8	2.3	1.7
Total CPU Time (hours)	20.6	19.5	18.9	20.7



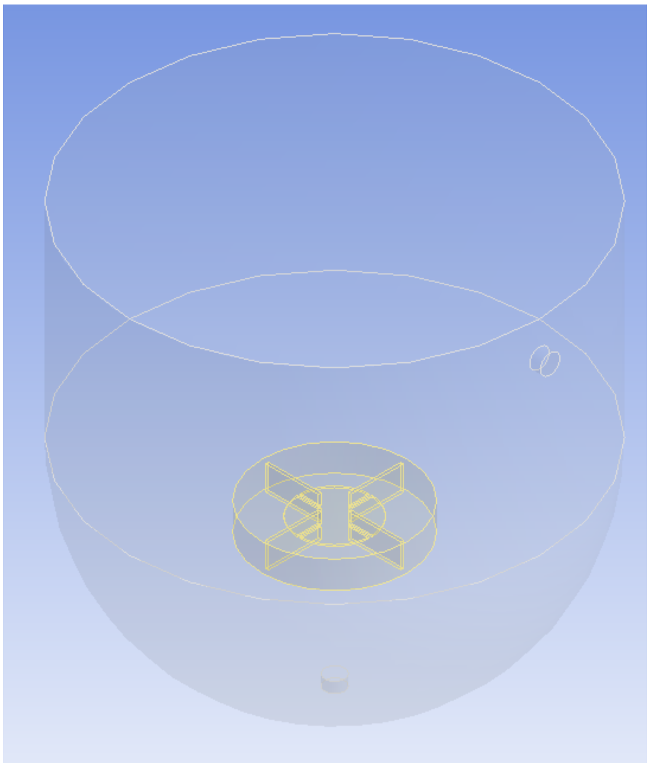
6 Biodiesel CSTR Example

6.1 Problem Statement

In this case we consider the simulation of a reaction within a CSTR vessel. The case will mimic the production of biodiesel (as methyl oleate) from a feed of methanol and a vegetable oil (modelled as pure triolein) through the simplified reversible reaction outlined below:

$$\underset{\text{Triolein}}{C_{57}H_{104}O_6} + \underset{\text{Methanol}}{CH_3OH} \overset{\text{NaOH}}{\rightleftharpoons} \underset{\text{Methyl oleate}}{C_{19}H_{36}O_2} + \underset{\text{Glycerol}}{C_3H_8O_3}$$

Hypothetical kinetic parameters are used to model the reaction in the absence of relevant kinetic data. The geometry of the vessel is shown below.



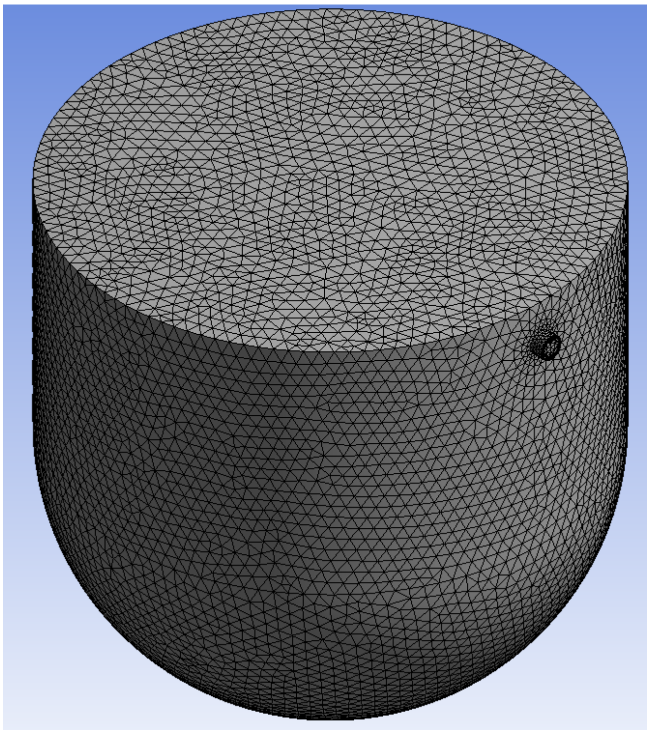
This geometry file can be found on ARCHIE at /opt/gridware/examples/fluent. The processing conditions are summarised in Table 10.

Table 10: Summary of process conditions

Vessel Volume /[m^3]	Agitator Type	Agitator Speed /[rpm]	Inlet Velocity /[$m.s^{-1}$]	Inlet Flowrate /[$L.s^{-1}$	Mass Fraction Triolien in	Inlet Temperature /[K]
14.63	Rushton turbine	100	0.4	5.68	0.2802	333.15

Due to the presence of high sheer in the fluid region surrounding the agitator it is likely that vortex shedding will occure close to the impeller. To account for the inherent unsteady nature of the system this system will be simulated using a transient regime. A two step procedure was used to effectively simulate the following reactive system. Firstly, an unreactive steady state simulation is carried out to set-up the approximate flow field within the vessel. Full convergence is not required at this stage (and is generally not achievable in steady state mode for such a case). Next the simulation is placed in transient mode, volumetric reactions are turned on and product species are tracked. The two parts of the simulation are submitted as a single job and the journal file performs the task modifying the set-up once the initial steady state simulation is completed.

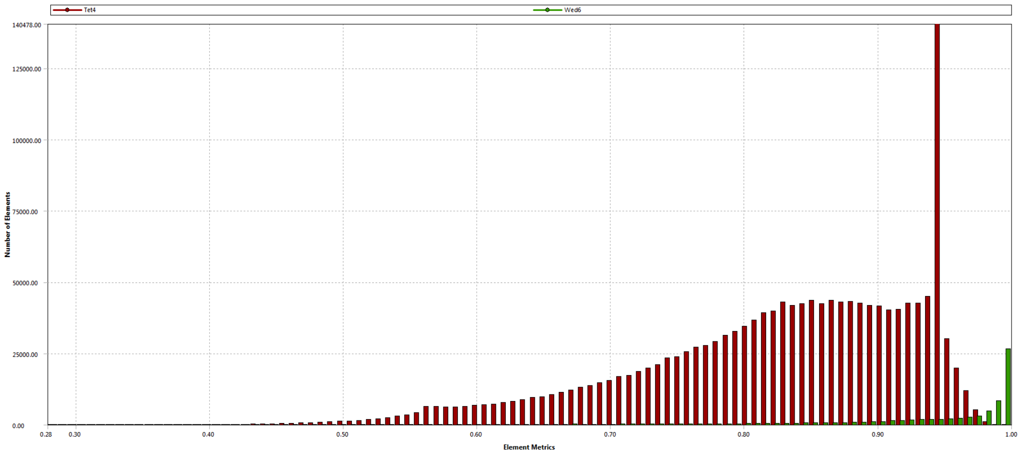
6.2 Details of The Mesh



Due to the complex nature of this design the number of elements required for effective simulation of the system is particularly large. The details of the resulting mesh are detailed in Table 11.

Table 11: Details of the mesh

Nodes	331879
Elements	1633444
Mesh Metric	Orthogonal Quality
Min	0.27873
Max	0.99995
Average	0.83209
Standard Dev.	0.10579
Approximate RAM usage	0.8GB



The mesh file can be found on ARCHIE at /opt/gridware/examples/fluent.

6.3 Details of the Local Fluent Set-up

The details of the Fluent set-up defined on the local machine prior to uploading to the ARCHIE system. For details of this set-up please see the .cas file which can be found on ARCHIE at /opt/gridware/examples/fluent.

6.4 ARCHIE Scripts

6.4.1 The Job Script

```
#!/bin/bash

module load apps/bin/fluent/15.0.1

# ************* SGE qsub options ****************
#Export env variables and keep current working directory
#$ -V -cwd
#Select parallel environment and number of parallel queue slots (cores)
#$ -pe multiway 4
#$ -P PROJECTNAME.prj
#Combine STDOUT/STDERR
#$ -j y
#Specify output file
#$ -o out.$JOB_ID.doc
#Request resource reservation (reserve slots on each scheduler run
#until enough have been gathered to run the job
#$ -R y
# Add runtime indication
#$ -ac runtime="14hr"
# ************** END SGE qsub options ************
```

```
#Initiating Fluent and reading .txt file
fluent 3d -pib -ssh -sge -g -i example_4_fluent_input.txt > output
```

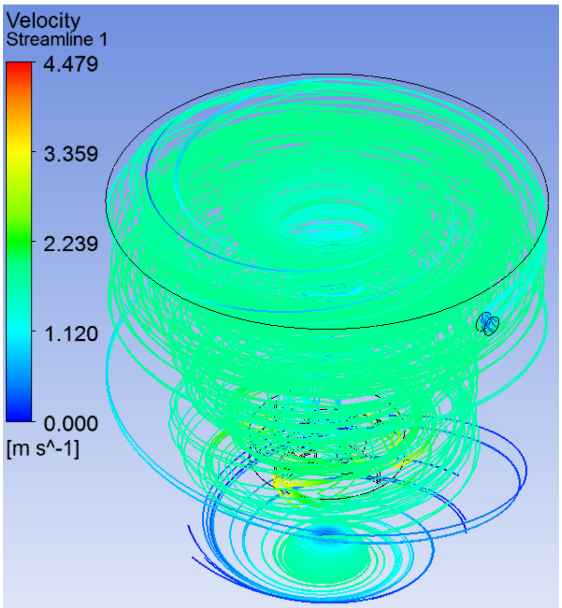
6.4.2 Fluent Input Script

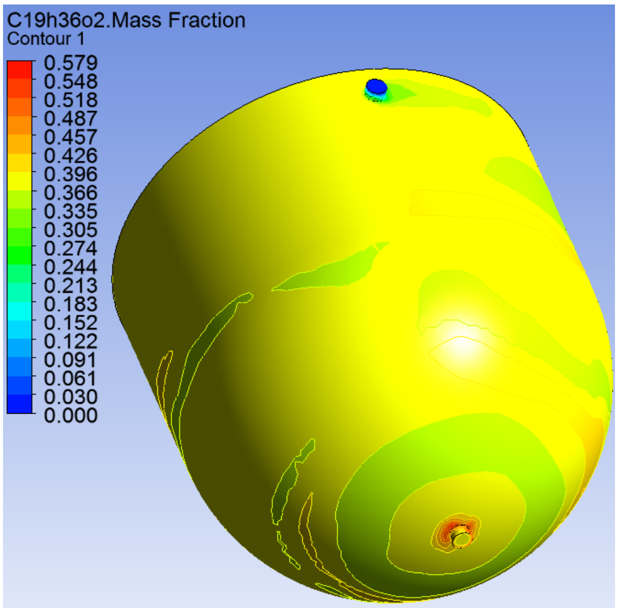
```
;Example 4:  Biodiesel CSTR
;
;Reading the case file
rc cstr_pre_reaction_setup.cas.gz
;
;Hybrid Initialising the system for non-reactive step
solve/init/hyb-init
;
;Setting the number of steady state iterations
solve/it/2000
;
;Writing the case file for the non-reactive
;flow field (overwriting if necessary)
wc pre_reaction_ff4.cas.gz
yes
;
;Writing the data file for the non-reactive
;flow field (overwriting if necessary)
wd pre_reaction_ff4.dat.gz
yes
;
;Reporting the performance of the non-reactive solver stage
parallel timer usage
;
;Setting the solver to transient mode for reactive step
define models unsteady-1 yes
;
;Turning on volumetric reactions
define/models/species/volumetric-reactions yes
;
;Defining the reaction solver method
define/models/species/set-turb-chem-interaction no no no yes
;
;Tracking product species
solve/set/equations/species-1 yes
solve/set/equations/species-2 yes
;
;
;Set the transient time-sep size (sec)
solve/set/time-step 0.01
;
;Set the number of time-steps (first number) and the
;max number of iterations per time-step (second number)
```

```
solve dual-time-iterate 1000 1000
;
;Reporting the performance of the combined simulation
;steps (non-reactive + reactive)
parallel timer usage
;
;Writing the post-reaction case file
wc post_reaction4.cas.gz
yes
;Writing the post reaction data file
wd post_reaction4.dat.gz
yes
;Exiting Fluent
exit
yes
```

6.5 Results

The following images were generated on a local machine within CFD Post using ARCHIE Fluent simulation data.



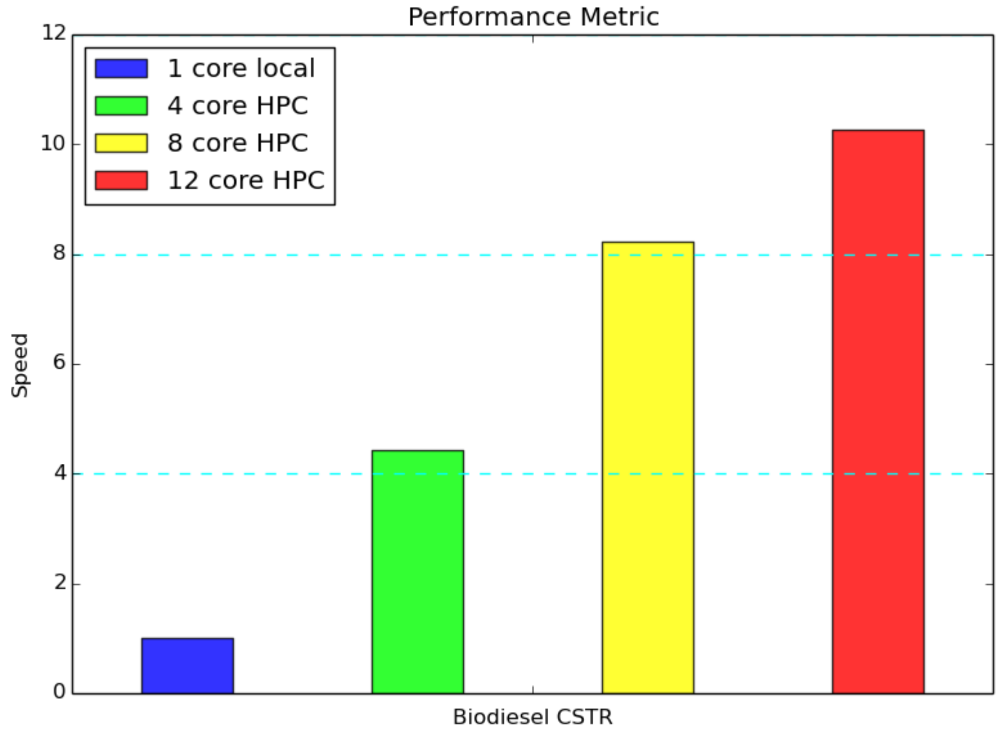


6.6 Performance

The simulation performance of each is detailed in Table 12 and the relative performance illustrated below.

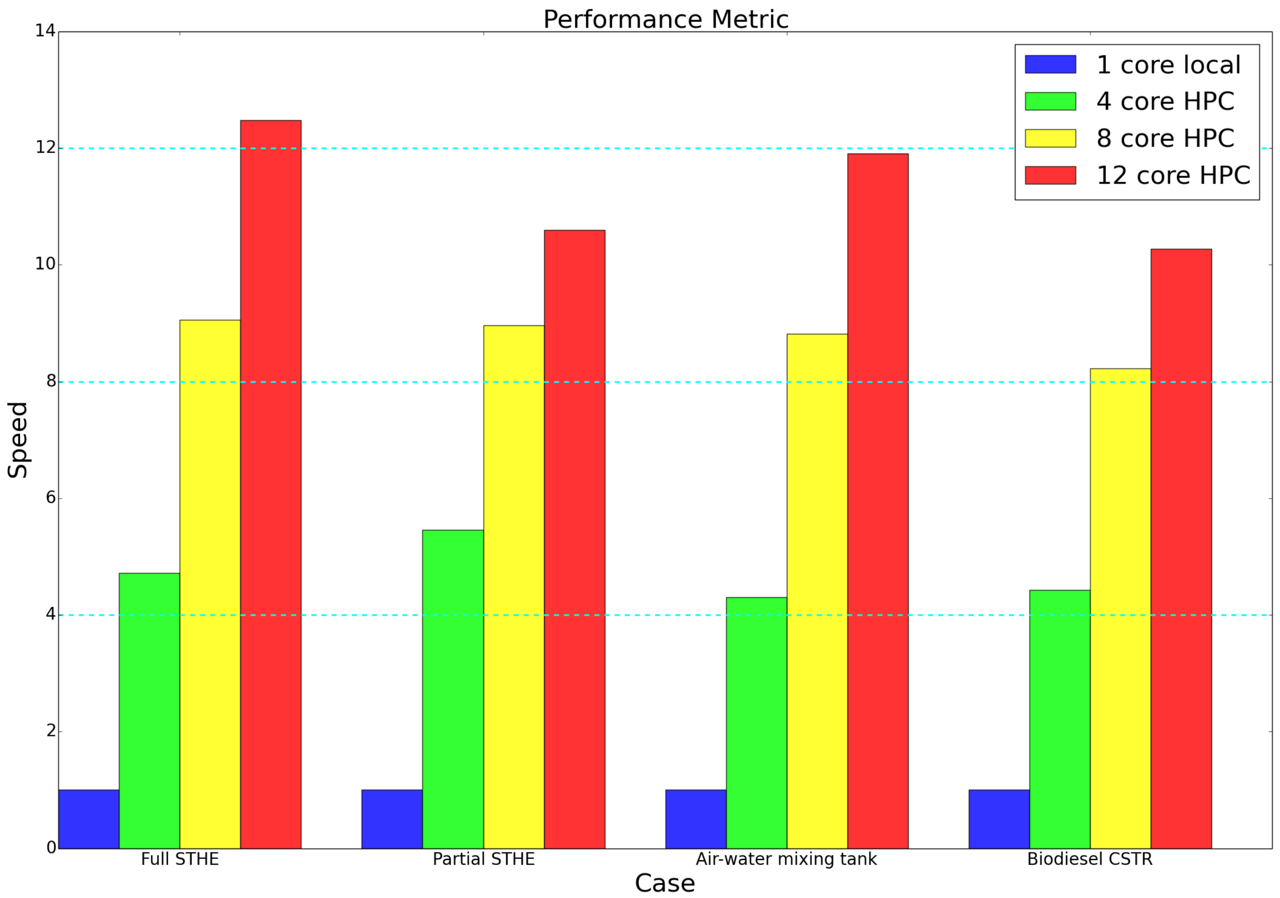
Table 12: Summary of performance over selected number of computing cores (ARCHIE HPC and local machine)

Number of Cores (System)	1 (Local)	4 (ARCHIE)	8 (ARCHIE)	12 (ARCHIE)
Simulation Wall-Clock Time (hours)	53.3	13.5	6.5	5.2
Total CPU Time (hours)	53.3	48.9	52.2	61.8



7 Performance Summary

Here we present a summary of the relative performance of all the simulations carried out for all examples in this manual.



8 Acknowledgements

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9 Appendix

The following procedure allows for the analysis of the history of a transient Fluent simulation.

9.1 Pre-simulation Fluent Set-up

File > Export > During Calculation > Solution Data
In the Automatic Export dialogue box:

- set *File Type* to *CFD Post compatible*
- select the desired quantities to be exported for analysis
- choose a frequency
- specify whether or not a case file is to be exported for each data set
- choose the output format (binary or askey)

9.2 Post Processing in CFD Post

- *File > Load Results*
- select *Load complete history as*
- select *a single case*
- click *Open*

The user may now create plots and animations in CFD Post at any point in the simulation history. Note that it is also possible to load cdat files in alternative third party post processing programs.