



zCFDguide Documentation

Release v2026.06.14267

Zenotech Ltd

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CONTENTS

1	Version: v2026.06.14267	1
1.1	Overview	1
1.2	Installation	1
1.3	Running zCFD	4
1.4	Getting Started	10
1.5	Reference Guide	54
1.6	zCFD Functions	121
1.7	Mesh Conversion	126
1.8	FWH solver	128
1.9	zM3	137
1.10	Visualisation	140
1.11	Utilities	143
1.12	Troubleshooting	145

VERSION: V2026.06.14267

1.1 Overview

zCFD is a GPU-accelerated high-performance computational fluid dynamics (CFD) solver.

zCFD is designed to make highly effective use of modern computer architectures. It is structured as a high performance core, executed via a flexible Python based wrapper. zCFD will run on unstructured meshes from a variety of sources, and will export data in many common formats. zCFD offers an easier route to coupling multi-disciplinary capabilities and integrating third-party data sources.

Features include both compressible and incompressible finite-volume formulations, overset capability and fluid-structure interaction (FSI) running on both CPUs and GPUs. zCFD is capable of performing both steady-state and time accurate simulations, with a range of time marching schemes. The numerical schemes available have been selected for accuracy and robustness. The code provides automatic scaling of turbulent wall functions; automatic determination of inflow / outflow conditions and pre-conditioning to allow for low and high Mach number flow.

zCFD makes use of the MPI protocol to manage execution over a set of compute nodes. The execution process is completely parallel from the start to finish including all the input/output functionality. To support this scalable implementation the mesh input is provided in hdf5 format which is portable and self describing. Filters are provided to convert the most frequently used formats to this internal format.

zCFD uses a single control dictionary to specify all the parameters. This is a Python file containing a python dictionary with certain mandatory keys. The use of Python for the control dictionary enables the user to add custom functions that populate the dictionary at runtime.

The zCFD distribution also ships with zm3 or zMesh-Cubed, our cartesian cut cell immersed boundary mesh generator. This allows users to rapidly generate meshes for CFD from STL files, with minimal user cleanup effort required.

1.2 Installation

1.2.1 System Requirements

zCFD is supported on the following Linux distributions:

- RHEL 7+
- CentOS 7+
- Ubuntu 20.04+
- Windows 10/11 via [WSL2](#)

By default zCFD is compiled for x86_64 but is available for ARM and IBM Power on request.

GPU support

zCFD supports running on NVidia GPUs with a compute capability of 6.1 and above (See [Compute Capability](#)).

An AMD GPU (HIP) based version is available on request.

1.2.2 Linux / Unix

If you are running Linux/Unix zCFD is provided as a stand-alone installer containing all the packages required to get started. The installer is available for download from the [zCFD website](#). Once the zCFD installer has been downloaded run the install script and follow the prompts.

```
$ bash zCFD-icx-sse-impi-<INSTALL_VERSION>-Linux-64bit.sh
```

Then copy the license file provided over email into the lic folder in the install directory.

```
$ cp zcfd.lic /<path to zCFD install>/lic/
```

Once zCFD has been installed the zCFD environment can be activated from a bash shell:

```
$ source /<path to zCFD install>/bin/activate  
(zCFD)$
```

1.2.3 Windows

zCFD can be run locally on windows machines if Windows Subsystem for Linux 2 (WSL2) is installed. To install WSL2 simply follow the Microsoft instructions which can be found [here](#).

The chosen Linux distribution shouldn't have an effect on how the code runs, but the Linux distributions listed above are supported.

In order to access your Linux filesystem on Windows it can be useful to add a quick access link in file explorer. To do this, in the address in file explorer enter

```
\\wsl$\
```

This will show you show you the root folders for your installed Linux distributions.

The installer is available for download from the [zCFD website](#). For WSL, download the standard Linux distribution. Once the zCFD installer has been downloaded run the install script from within the WSL2 environment and follow the prompts.

```
$ bash zCFD-icc-sse-impi-<INSTALL_VERSION>-Linux-64bit.sh
```

Then copy the license file provided over email into the lic folder in the install directory.

```
$ cp zcfd.lic /<path to zCFD install>/lic/
```

Once zCFD has been installed the zCFD environment can be activated:

```
$ source /<path to zCFD install>/bin/activate  
(zCFD)$
```

1.2.4 Licence

zCFD requires a license. If you do not already have a license, please contact zcf@zenotech.com to obtain one. When zCFD starts it will look in the following locations for a licence file:

1. 'zcfd.lic' in the directory alongside the input files
2. 'zcfd.lic' in the lic directory of the zCFD installation. i.e. /<path to zCFD install>/lic/

3. RLM_LICENSE environment variable

The RLM_LICENSE environment variable can be defined as below.

```
export RLM_LICENSE=/path/to/license/file
```

or, where port is the port number in the license file, and host is the hostname in the license file

```
export RLM_LICENSE=port@server
```

In the case that the system running the simulation cannot access the internet a local license server will be required. See <http://www.reprisesoftware.com/admin/software-licensing.php> for details.

Licence Error codes

Below is a list of some of the error codes that you may encounter due to licensing errors. If the error code you receive is not listed, please see RLM's documentation a <https://reprisesoftware.com/docs/isv/appendix/appendix-b-rlm-status-values.html> or contact us.

Error Code	Description	Possible Remedy
-3	License has expired	Contact us to renew your license
-6	Requested version is not supported	Your license is for an older product version; contact us to upgrade
-8	checkout request for too many licenses	Reduce the number of ranks that you are running the solver on or stop any existing running processes.
-17	Error communicating with server	There was a connectivity issue connecting to the license server. Check that you have connectivity to the license server; check firewall settings and any endpoint security software you may be running
-21	No heartbeat	The license heartbeat was not received; check that the license server is still running and that have connectivity to it
-22	All licenses in use	All licenses are currently in use; stop any running processes to free up a license.
-37	License start date has not been reached	Your license has not yet become valid. Contact us if you believe this to be in error
-102	Can't read license data	Check the permissions on the license file on the server
-103	Network error	Check that you have connectivity to the license server; this may involve opening a port on your firewall or connecting to the internet
-104	Error writing to network	Check your connectivity to the license server; check firewall settings and any endpoint security software you may be running
-105	Error reading from network	Check your connectivity to the license server; check firewall settings and any endpoint security software you may be running
-106	Unexpected response from license server	Check that your license configuration is pointing to the correct server
-107	HELLO message for wrong server	Check that your license configuration is pointing to the correct server
-108	Error in private key	There is an issue with your server side license file - contact us to resolve this issue
-109	Error signing authorization	There is an issue with your server side license file - contact us to resolve this issue

continues on next page

Table 1.1 – continued from previous page

Error Code	Description	Possible Remedy
-110	Internal error	An error occurred in the license server - contact us if this error repeats itself
-111	Connection refused at server	Check your firewall settings and that you are pointing at the correct license server
-112	No server to connect to	Check that the server is running and that you are pointing at the correct license server
-113	Bad Communication handshake	Check that the server is running and that you are pointing at the correct license server
-114	Can't get ethernet address	Check that the user that you are running as has correct permissions to query the network card

1.3 Running zCFD

zCFD is primarily run from the command line, you can run on your local machine or submit it to a batch scheduler for parallel execution. The following sections give information on how to execute zCFD.

1.3.1 Running zCFD

zCFD is designed to exploit parallelism in the target computing hardware, making use of multiple processes (MPI), multiple threads per CPU process (OpenMP) and / or many threads per GPU. zCFD will handle most parallel functions automatically, so the user just needs to specify how much, and what type, of resource to use for a given run.

Table of Contents

- [Command Line Execution](#)
- [Input Validation](#)
- [Overriding Mesh and Case Names](#)
- [Batch Queue Submission](#)

Command Line Execution

zCFD includes an in-built command-line environment, which should be activated either when run directly or via a cluster management and job scheduling system, such as Slurm.

```
source /INSTALL_LOCATION/zCFD-version/bin/activate
```

This sets up the environment to enable execution of the specific version. When within the command-line environment, the command prompt will show a zCFD prefix:

```
(zCFD) >
```

To deactivate the command line environment, returning the environment to the previous state use:

```
deactivate
```

Your command prompt should return to its normal appearance.

To run zCFD on the command-line:

```
run_zcfd -n <num_tasks> -d <device_type> -p <mesh_name> -c <case_name>
```

where:

Parameter	Value	Description
num_tasks	Integer	The number of partitions (one per device socket - CPU or GPU)
device_type	CPU or GPU	Specifies whether or not to use GPU(s) if present
mesh_name	String	The name of the mesh file (<mesh>.h5)
case_name	String	The name of the control dictionary (<control_dict>.py)

For example, to run zCFD from the command-line environment on a desktop computer with a single 12-core CPU processor and no GPU:

```
run_zcfd -n 1 -d cpu -p <mesh_name> -c <case_name>
```

By default, zCFD will use all 12 cores via OpenMP unless a specific number is required. To run the above case using only 6 cores (there will be one thread per CPU core):

```
run_zcfd -n 1 -d cpu -o 6 -p <mesh_name> -c <case_name>
```

or

```
export OMP_NUM_THREADS=6; run_zcfd -n 1 -d cpu -p <mesh_name> -c <case_name>
```

To run zCFD on a desktop computer with a single CPU and two GPUs:

```
run_zcfd -n 2 -d gpu -p <mesh_name> -c <case_name>
```

Input Validation

zCFD provides an input validation script which can be used to check the solver control dictionary before run time reducing the likelihood of a job spending a long time queuing only to fail at start up.

The script can be executed from the zCFD environment as follows:

```
validate_input <case_name> [-m <mesh_name>]
```

If the -m option is given with a mesh file the script will check whether any zones specified as lists to boundary conditions, transforms or reports in the input exist in the mesh.

Overriding Mesh and Case Names

For more advanced simulations with overset meshes (see *overset*) an override dictionary can be supplied as an additional argument to the command-line, in interactive mode or within a batch submission script, to specify multiple meshes and associated control dictionaries:

```
run_zcfd -n 2 -d gpu -f <override_file>
```

An example override.py file for a background domain with a single rotating turbine would be:

```
override = {'mesh_case_pair': [( 'background.h5', 'background.py'),
                               ( 'turbine.h5', 'turbine.py')]}
```

Batch Queue Submission

To run zCFD on a compute cluster with a queuing system (such as Slurm), the command-line environment activation is included within the submission script:

Example Slurm submission script “run_zcfd.sub”:

```
#!/bin/bash
#SBATCH -J account_name
#SBATCH --output zcf.d.out
#SBATCH --nodes 2
#SBATCH --ntasks 4
#SBATCH --exclusive
#SBATCH --time=10:00:00
#SBATCH --gres=gpu:2
#SBATCH --cpus-per-task=16
source /INSTALL_LOCATION/zCFD-version/bin/activate
run_zcfd -n 4 -d gpu -p <mesh_name> -c <case_name>
```

In this system we have 2 nodes, each with 2 GPUs. We allocate one task per GPU, giving a total of 4 tasks. Note that `num_tasks`, in this case 4, on the last line should match Slurm “ntasks” on line 5. The case is run in “exclusive” mode which means that zCFD has uncontested use of the devices. In this case we have a 64-core CPU, giving 16 CPU cores for each of the 4 tasks. The “gres” line tells zCFD that there are 2 GPUs available on each node.

The submission script would be submitted from the command-line:

```
sbatch run_zcfd.sub
```

The job can then be managed using the standard Slurm commands.

Note

Users unfamiliar with the batch submission parameters in a specific system should consult the system administrator.

1.3.2 Parallel Guide

Concepts

zCFD uses Intel MPI (Message Passing Interface) to enable running over multiple machines or multiple GPUs, either in one machine or across multiple. A paid license is required for this functionality. This is achieved by decomposing the domain into parallel regions that are distributed to each MPI rank. MPI can leverage high bandwidth network interconnects such as infiniband or AWS’ Elastic Fabric adaptor,

There are two main strategies for running the code in parallel:

Hybrid MPI/OpenMP runs one MPI process per socket, reducing the number of MPI ranks at larger core counts. Running in hybrid mode assigns multiple cores to each MPI rank, allowing it to reduce the communication overheads associated with running in parallel.

Full MPI runs one MPI process per core and is typically the best strategy for low core count runs or GPU based runs. For GPU runs, you can run 1 MPI rank per GPU available on the node, or multiple MPI ranks per GPU. When running multiple ranks per GPU, the ranks will share the GPU resources. This can be useful for smaller problem sizes, testing and development, or workloads with low GPU utilization.

To run in parallel you add the `-n` option to the `run_zcfd` script. The provided argument is the number of MPI processes to launch.

Hybrid MPI/OpenMP

This is the default mode for zCFD. It will auto detect the number of sockets on each node and set the number of OpenMP threads appropriately. The `-tpn` option to `run_zcfd` can be used to set the number of MPI processes to launch on each node. The number of OpenMP threads will be set automatically by dividing the total number of cores between all processes.

For example, if you had two hosts with 2 x 12 core CPUs per host and you wanted to run Hybrid MPI/OpenMP you would request 1 MPI rank per CPU socket and zCFD will automatically set the number of OpenMP threads per rank to match the number of cores per socket (in our case 12).

```
run_zcfd -m <mesh_name> -c <case_name> -n 4 -tpn 2
```

The number of OpenMP threads assigned to each rank can be overridden by setting **OMP_NUM_THREADS** in the calling environment.

Full MPI

This is achieved by running zCFD with **OMP_NUM_THREADS** set to 1 and passing `-n <tasks>` where `tasks` is the number of MPI ranks.

For example, if you had two hosts with 2 x 12 core CPUs per host and wanted to run full MPI with 1 MPI rank per core you could do the following:

```
export OMP_NUM_THREADS=1
run_zcfd -p <mesh_name> -c <case_name> -n 48 -tpn 24
```

GPU Parallel Execution

zCFD automatically assigns GPUs to MPI ranks when running on GPU-enabled nodes.

Single Rank per GPU: This is the default and recommended configuration for most workloads. Each MPI rank gets exclusive access to one GPU.

```
# For a node with 4 GPUs, run 4 ranks (1 per GPU)
run_zcfd -p <mesh_name> -c <case_name> -n 4
```

Multiple Ranks per GPU (Experimental): To enable multiple MPI ranks sharing GPUs, set the `ZCFD_DEV_OVERSUBSCRIBE_GPU` environment variable. This is an experimental feature primarily intended for debugging and testing. When enabled, ranks will be assigned to GPUs using modulo arithmetic (`rank % num_gpus`).

Warning

GPU oversubscription is an experimental feature. It may result in reduced performance and is primarily intended for debugging purposes with limited GPU resources.

This can be useful for:

- Testing and development with limited GPU resources
- Debugging with smaller problem sizes
- Workloads with low GPU compute utilization

```
# For a node with 4 GPUs, run 8 ranks (2 per GPU) - experimental
export ZCFD_DEV_OVERSUBSCRIBE_GPU=1
run_zcfd -p <mesh_name> -c <case_name> -n 8
```

Example assignments with oversubscription enabled:

- 4 GPUs, 4 ranks: GPU assignment [0,1,2,3]
- 4 GPUs, 8 ranks: GPU assignment [0,1,2,3,0,1,2,3]
- 4 GPUs, 6 ranks: GPU assignment [0,1,2,3,0,1]

Running across multiple machines with a cluster scheduler

There are many cluster scheduling systems but commonly used ones are Slurm, PBS Pro or GridEngine. Please refer to either the cluster scheduling software or your local HPC systems' documentation for how to submit jobs to the appropriate nodes on your system as configuration varies between machines.

Intel MPI has tight integration to most commonly used scheduling systems and so will typically autodetect the nodes to run on.

Running across multiple machines without a cluster scheduler

If your cluster does not have a scheduling system then `I_MPI_HYDRA_HOST_FILE` can be set in the environment to point at a file containing the list of hostnames that zCFD will launch on. For example:

```
export I_MPI_HYDRA_HOST_FILE=~/.hosts.file
```

Note

For this to run you need to be able to ssh without a password to each of the machines listed.

An example contents of a hosts file is shown below:

```
Compute01:2  
compute02:2  
Compute03:1
```

This file specifies three hosts, compute01, compute02, compute03 where 2 ranks will be launched on each of compute01 and compute02 and 1 rank will be launched on compute03.

Alternatively this could be specified as which would launch processes round robin through the list of machines listed in the file.

```
Compute01  
compute02  
Compute03
```

Libfabric provider selection

zCFD will attempt to autodetect the correct provider to use for MPI communication. It tries the following providers in order:

```
efa  
psm2  
mlx  
verbs  
tcp  
sockets
```

If `FI_PROVIDER` is set then the autodetection is skipped.

Using cluster provided libfabric

By default zCFD will use the version of libfabric that ships with Intel MPI. For some advanced use cases you may wish to make use of preinstalled libfabric. This may be if you have a custom network driver or a specific configuration on your cluster. To enable this then set the `I_MPI_OFI_LIBRARY_INTERNAL` environment variable to 0

```
export I_MPI_OFI_LIBRARY_INTERNAL=0
```

Pre launch script

On some systems the defaults setup by zcfid may not be optimal and so a custom script to modify the environment can be injected by setting the environment variable **ZCFD_PRE_LAUNCH** to the path to a script. This script will be sourced from within a bash environment just before the solver is launched.

An example use case for this is to bind a GPU to a specific network interface on a multi-homed network system.

OpenMP affinity

By default zCFD binds its OpenMP threads to cores using the **OMP_PROC_BIND** and **OMP_PLACES** environment variables.

Other MPI implementations

On platforms where Intel MPI doesn't work then we can build zCFD against a specific implementation of MPI. This would be a custom deployment for your facility so get in touch with us if you need this.

Running at large scale

As zCFD is partly written in python, the install consists of a large quantity of small files, which on a large scale cluster can have a negative impact on the cluster filesystem during startup. In order to mitigate this it is possible to stage the code into either local storage or memory on the compute nodes using MPI to broadcast the data.

Contact us if you want to run in this mode.

1.3.3 Using Jupyter

We also recommend the use of [Jupyter Notebooks](#) for post-processing zCFD runs. This is one of the easiest ways to use Python, via an interactive notebook on your local computer. The notebook is a locally hosted server that you can access via a web-browser. Jupyter is included in the zCFD distribution and notebooks for visualising the residual data will automatically be created when you run a zCFD case.

To automatically start up notebook server on your computer within the zCFD environment run:

```
start_lab
```

The output of the command will include the URL to Jupyter is running on, simply copy and paste this into your browser to connect to Jupyter. To stop Jupyter use *Ctrl + c* in the terminal where Jupyter is running.

1.3.4 zCFD Environment Variables

The following table gives some of the environment variables that can be set before running zCFD. These are generally for advanced users can can impact the way zCFD runs on you system.

Variable	Default	Description
ZCFD_GPUDIREC	unset	Set if you are using NVIDIA GPU direct (custom builds only) with a CUDA aware mpi implementation.
ZCFD_PRE_LAUN	unset	This option allows a script to be run just before the code is launched so that the user can override any environment that has been automatically setup.
CUDA_VISIBLE_D	unset	This option restricts the list of GPU devices that zCFD will be able to use. Typically this can be used to remove an incompatible GPU or the display GPU from the list of candidate GPUs.
ZCFD_DISABLE_P	unset	When set this causes the GPU memory allocated to be page-able and not pinned memory. This should always be used on Windows in WSL as CUDA inside WSL has a fixed low threshold for the maximum amount of allowed pinned memory.
ZCFD_NCCL	unset	Set to 1 to make use of the NVIDIA NCCL library during parallel exchanges.
PMPI_CUDA	unset	Set if you are running with platform MPI (custom builds only) to enable GPU aware MPI memory allocations
MPICH_GPU_SUF	unset	Set to 1 if you are running with Cray MPI (custom builds only) to enable GPU aware MPI memory allocations
ZCFD_DISPATCH	unset	Makes all kernel launches synchronous.
ZCFD_DEV_OVER	unset	Experimental feature. When set, allows multiple MPI ranks to share the same GPU. Without this variable set, the default behavior assigns one GPU per MPI rank. This is primarily intended for debugging and testing with limited GPU resources.

1.4 Getting Started

The getting started guide is here to teach the fundamentals of using zCFD, starting with a simple case and building up the complexity of the simulation. These should provide you a good starting point for setting up your own simulations. All of the input files required for the guide are available on line.

1.4.1 Tutorial 1: Simple Aerofoil

Table of Contents

- *What is in this tutorial?*
- *What you need?*
- *Step 1. Download the files*
- *Step 2. Review Control file*
 - *Time marching*
 - *Equations*
 - *IC_1*
 - *BC_1*
 - *BC_2*
 - *BC_3*
 - *Report*
 - *Write Output*

- *Step 3. Running zCFD*
- *Step 4. Review the output*
- *Step 5. Looking at residuals with notebook*
 - *Plotting residuals*
 - *Plotting forces*
 - *Plotting performance*
- *Step 6. Looking at results with Paraview*
 - *Loading your data*
 - *Visualising Variables*
 - *Pressure Coefficient Plot*

What is in this tutorial?

The NACA0012 is a symmetrical aerofoil which is commonly used for code validation. In this configuration it is a quick and simple simulation to run. By downloading this [zip file](#) and following the instructions below, you should learn to run, post-process and visualise a simple zCFD simulation. This is a small simulation which most users should be able to run on a laptop in ~5 minutes.

What you need?

To run the tutorial you will need an installation of zCFD and a valid licence (the free licence is sufficient for this tutorial). For instructions on installing zCFD please see [here](#).

The tutorial assumes that you are running all commands using a bash shell on Linux.

Step 1. Download the files

The tutorial zip file can be downloaded [here](#). The zip file contains a mesh file (*naca0012.h5*) and a zCFD control file (*naca0012.py*).

This tutorial will assume you unzip the file in a directory called “zcf_tutorial_1” in your users home directory.

```
cd ~
mkdir zcf_tutorial_1
wget https://zcf.zenotech.com/tutorials/1/naca0012.zip
unzip naca0012.zip
```

Step 2. Review Control file

naca0012.py is the zCFD control file. When we run zCFD, zCFD reads the control file and uses the Python dictionary parameters to set the solver settings. A brief overview of the parameters dictionary for the simulation is given below; for a more detailed description of the control file structure, see the [reference guide](#).

```
parameters = {
    "time marching": {
        "unsteady": {"total time": 1.0, "time step": 1.0},
        "scheme": {"name": "implicit euler", "stage": 1},
        "cfl": 50,
        "cfl ramp factor": {"growth": 1.1, "initial": 1.0},
        "cycles": 1500,
    },
    "equations": "RANS",
    "RANS": {
        "order": "euler_second",
```

```
    "turbulence": {"model": "sst"},
    "inviscid flux scheme": "Roe",
  },
  "IC_1": {
    "temperature": 300,
    "pressure": 101325.0,
    "V": {"vector": [1.0,0.0,0.0], "Mach": 0.15},
    "viscosity": 1.02145e-05,
    "turbulence intensity": 5.2e-2,
    "eddy viscosity ratio": 1.0,
  },
  "BC_1": {
    "zone": [1],
    "type": "farfield",
    "condition": "IC_1",
    "kind": "riemann",
  },
  "BC_2": {
    "zone": [4],
    "type": "wall",
    "kind": "noslip",
  },
  "BC_3": {
    "zone": [2, 3],
    "type": "symmetry",
  },
  "report": {
    "frequency": 10,
    "forces": {
      "FR_1": {"name": "wall", "zone": [4]},
    }
  },
  "reference": "IC_1",
  "write output": {
    "surface variables": ["V","p","mach","cp","cf","pressureforce",
- "frictionforce"],
    "volume variables": ["V", "p", "T", "rho", "mach", "cp", "eddy"],
  },
}
```

Time marching

The start of the parameters dictionary contains the *time marching* sub-dictionary. The *unsteady* sub-dictionary sets whether we are running an *unsteady* or a *steady* simulation. The fact that *total time* and *time step* are the same number means that we're running a steady simulation. Steady simulations assume that the flow we are simulating does not vary with time. Most real flows are not truly 'steady', but steady simulations tend to be much easier and cheaper to run than unsteady simulations. For an attached, streamlined flow like this one using a steady simulation is reasonable when time-resolved data is not required.

CFD simulations work by iteration - we start with a very rough estimate of the flow $f(x,0)$, then during the first 'iteration cycle' the solver uses $f(x,0)$ to create a better approximation of the flow, $f(x,1)$. This is repeated many times - we use $f(x,1)$ to calculate $f(x,2)$, $f(x,2)$ to calculate $f(x,3)$ and so on, until eventually we reach an estimate of the flow we are happy with.

The flow will generally change very quickly in the first few iterations, and then converge asymptotically on the 'right' answer. The *cycles* parameter states how many iterations should be used in the simulation - the higher it is the more accurate the solution is likely to be, but given the convergence is asymptotic setting it too high will lead to lots of computational effort being used for very little change in the solution towards the end.

The *scheme* defines the numerical scheme used by the solver to get from $f(x,n)$ to $f(x,n+1)$. The *implicit*

euler scheme is a sensible choice to use for this type of simulation.

The *CFL* essentially sets how much the flow is allowed to change between $f(x, n)$ and $f(x, n+1)$ approximations of the flow field - if it is set too high the simulation will not converge, and if it is set too low the simulation will take many cycles reach the appropriate flow.

Equations

The *equations* sets the type of flow we are simulating - there are a number of different options depending on the assumptions we make about the flow. *RANS* is used when we are simulating a compressible flow, and want to simulate the effects of turbulence on the mean flow by use of a turbulence equation. The *order* sets how the flow is spatially discretised, and the *turbulence* sets the turbulence model used.

IC_1

Now that the numerical settings have been defined, the flow needs to have boundary conditions. Boundary conditions define what happens at exterior faces of the mesh. In this case, there are three boundary conditions.

The first boundary condition we consider is that of the freestream air, which is at a temperature of 300 K, a pressure of 101325 Pa and flows parallel to the mesh's x axis at a Mach number of 0.15. The *IC_1* dictionary defines a flow at these conditions.

Because the RANS equations include the effect of viscosity, we also need to define the viscosity at the *IC_1* flow condition (in this case, we set it to be $1.02145 \times 10^{-5} \text{ kg m}^{-1} \text{ s}^{-1}$ at 300 K). This corresponds to a chord based Reynolds number of 6 million. Because the RANS equations include turbulence modelling, we also need to set the *turbulence intensity* and *eddy viscosity ratio* - these are used as boundary conditions for the SST turbulence model equations. The values given are sensible values for flows without significant freestream turbulence.

BC_1

The *BC_1* dictionary assigns the *IC_1* flow condition to all mesh faces contained in the mesh zone 1. Mesh zones are defined during the meshing process, and in this case mesh zone 1 contains all the mesh faces which are on the farfield exterior surface of the mesh. The *farfield* type means that flow can pass freely through the specified mesh faces, and the *riemann* kind means that flow can pass both in and out of the mesh via the specified mesh faces.

The *IC_1* dictionary is, by default, also used to define the initial guess for the flow - at 0 cycles we assume that the entirety of the flow is flowing at the *IC_1* conditions.

BC_2

The *BC_2* dictionary assigns a no-slip wall boundary condition to all mesh faces contained in the mesh zone 4. Mesh zone 4, in this case, contains all faces on the aerofoil surface.

BC_3

The *BC_3* dictionary assigns a symmetry boundary condition to all mesh faces contained in mesh zones 2 and 3, which are the +ve z and -ve z faces of the mesh. This boundary condition type is used here so that we can simulate an aerofoil of effectively infinite span, but with a low mesh resolution in the z axis to reduce simulation cost.

Report

The *report* dictionary defines which flow statistics zCFD should output to the user during the simulation, and how often. The 'frequency' key here defines that zCFD should report flow statistics to the user every 10 iteration cycles during the simulation. Exactly which flow statistics are outputted can be changed by the user, but the defaults should be enough for us to successfully monitor the convergence of the solution. The 'forces' sub-dictionary allows us to monitor the forces on specific mesh zones- here we are outputting the forces on mesh zone 1, which is the aerofoil surface. Some of the flow statistics (e.g. force on the aerofoil wall) are non-dimensionalised (see [here](#)) and the *reference* parameter defines the flow state they should be non-dimensionalised against. This is normally chosen to be the freestream state.

Write Output

The final section of *parameters*, *write output*, defines which variables should be outputted into VTK format for visualisation by the user at the end of the simulation.

Step 3. Running zCFD

To run zCFD you first need to source the “activate” script and then use the “run_zcfd” path.

1. Activating your environment:

```
source ./<ZCFD_INSTALL_PATH>/bin/activate
```

2. Run zCFD validate input to check the control dictionary for errors:

```
cd ~/zcfid_tutorial_1/
validate_input naca0012.py -m naca0012.h5
```

3. Run zCFD in the case directory:

```
run_zcfd -m naca0012.h5 -c naca0012.py
```

zCFD will attempt to detect the number of CPU cores and any GPUs present and make use of them. If you want to manually configure this see [here](#).

As the solver is running it will output information about the current CFL, Multigrid level, timing, reporting information and file I/O. The output from zCFD will be written to the screen and also to a log file “naca0012.log”.

```

Total Iterations: 2
Avg Convergence Rate: 0.0017
Final Residual: 1.368766e-07
Total Reduction in Residual: 3.047538e-06
Maximum Memory Usage: 1.541 GB
-----
Total Times: 0.0204855
setup: 0.0145224 s
solve: 0.0059631 s
solve(per iteration): 0.00298155 s
Timer: Elapsed seconds: 0.112
Breakdown of time spent:
output: 0 days 0 hrs 0 mins 0 s (count: 1499 cycles, avg: 0.0 ms)
reporting: 0 days 0 hrs 0 mins 2 s (count: 1499 cycles, avg: 1.5 ms)
solving: 0 days 0 hrs 3 mins 49 s (count: 1499 cycles, avg: 152.8 ms)
update source terms: 0 days 0 hrs 0 mins 0 s (count: 1499 cycles, avg: 0.1 ms)
cycle 1500 (real time cycle: 0 time: 0)
CFL: 50 (CFL-0) - MG: 50.0 (Coarse mesh: 0)
-----
iter Mem Usage (GB) residual rate
-----
Ini 1.54065 1.114668e-06
0 1.54065 1.823795e-07 0.1642
1 1.5406 6.884949e-08 0.3763
2 1.5406 3.105055e-08 0.4510
3 1.5406 1.744656e-08 0.5619
4 1.5406 1.028472e-08 0.5895
5 1.5406 6.720924e-09 0.6535
6 1.5406 4.63131e-09 0.6879
7 1.5406 2.735840e-09 0.5923
8 1.5406 1.637551e-09 0.5986
9 1.5406 9.747638e-10 0.5953
-----
Total Iterations: 10
Avg Convergence Rate: 0.4945
Final Residual: 9.747638e-10
Total Reduction in Residual: 8.744878e-04
Maximum Memory Usage: 1.541 GB
-----
Total Times: 0.072332
setup: 0.016222 s
solve: 0.0561101 s
solve(per iteration): 0.00561101 s
iter Mem Usage (GB) residual rate
-----
Ini 1.54065 4.622099e-02
0 1.54065 3.798742e-05 0.0008
1 1.5406 1.755518e-07 0.0046
-----
Total Iterations: 2
Avg Convergence Rate: 0.0019
Final Residual: 1.755518e-07
Total Reduction in Residual: 3.798097e-06
Maximum Memory Usage: 1.541 GB
-----
Total Times: 0.0203858
setup: 0.0145838 s
solve: 0.00580198 s
solve(per iteration): 0.00290099 s
Report: rho 0.00459256
Report: rho[U] 0.095179
Report: rho[V] 1.17148e-13
Report: rho[C] 0.00150043
Report: rhoE 0.0181309
Report: rhoK 0.000218339
Report: rhoT 0.00000000
-----
Checkpoint: Iters: 1500
Writing file naca0012_results.h5
Surface Data Field Output @ 1500
Writing VTK Surface Output
Volume Data Field Output @ 1500
Writing VTK Volume Output

```

Per cycle information
(exact format varies with time stepping
and compute device settings)

Writing report

Writing output information

zCFD will run for the 1500 *cycles* specified in the control dictionary, if you want to stop the solver early then you can either press CTRL+C to kill the process or update the *cycles* keyword to be a value smaller than the current cycle number, zCFD will detect this change and stop the solver.

The solver should take a few minutes to complete on a modern GPU, and a bit longer on a CPU.

Step 4. Review the output

A successful zCFD run will result in the following files and directories being created. In this case, since our control file is called *naca0012.py* the output files will also be created with that name. The `_OUTPUT` folder also includes an indication of the number of parallel partitions used, this tutorial assumes a single partition and so the output will be “naca0012_P1_OUTPUT” if we ran on two partitions it would be “naca0012_P2_OUTPUT”

File/Directory	Description
naca0012.log	This is simply a copy of the output to screen (see above) which happened during the run.
naca0012_report.csv	A .csv format table which shows the variation of flow statistics with cycle number
naca0012_report.ipynb	An auto-generated Jupyter notebook which can be used to read the naca0012_report.csv file and easily plot the flow statistics varying with cycle number.
naca0012_results.h5	The flow solution calculated by zCFD, in zCFD format. This can be used for visualisation, but it is generally only used for restarting zCFD simulations from
naca0012_status.txt	A .json format file outputted by zCFD. Among other things, it records when the simulation was last run, which mesh was used and which control file was used.
naca0012_P1_OUTPUT/	A directory which contains flow solution calculated by zCFD, in VTK format. This is generally more suitable for visualising the data with than the zCFD proprietary format.
naca0012_P1_OUTPUT/naca0012_results.h5	A VTK file which, when opened, will load all the volume data from the simulation.
naca0012_P1_OUTPUT/naca0012_wall.pvd etc	A series of VTK files (one for each boundary condition type) which, when opened, will load the surface data for that boundary condition.
naca0012_P1_OUTPUT/VISUALIZATION/	Contains the raw data files which are loaded when the naca0012.pvd and naca0012_farfield.pvd, naca0012_wall.pvd etc. files are opened.
naca0012_P1_OUTPUT/LOGGING/	Contains a separate copy of the naca0012.log file for each MPI partition. Used for debugging.

Step 5. Looking at residuals with notebook

The naca0012_report.ipynb file can be loaded using a variety of methods, but here we will load it using a browser. The commands below should open Jupyter Notebook within a browser window. If the browser does not open automatically then the notebook URL should be visible in the command output.

1. Activate your environment:

```
./<ZCFD_INSTALL_PATH>/bin/activate
```

2. Start the Jupyter Notebook:

```
cd ~/zcf_d_tutorial_1/
start_lab
```

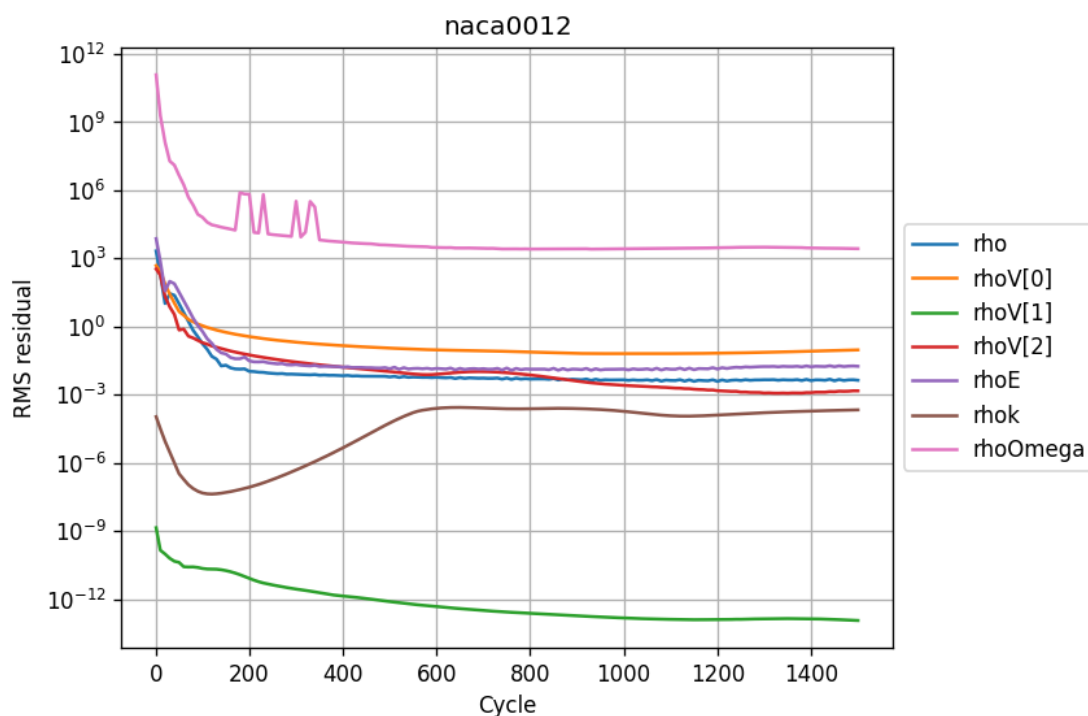
Load the naca0012_report.ipynb in Jupyter, then click run `all`.

Plotting residuals

The naca0012_report.ipynb makes use of the `zutil.plot.zcf_d_plots` function to read and plot the zCFD report data. Calling the `zcf_d_plots('naca0012.py')` function reads the zcf_d control file, finds all the output files, and returns a `zutil.post.Report` object, which provides plotting functionality. To plot the convergence of residuals, use the `plot_residuals()` method:

```
from zutil.plot import zcfd_plots
r = zcfd_plots('naca0012.py')
r.plot_residuals()
```

The residual variables essentially measure how close to a stable solution of the chosen flow equations (e.g. the RANS equations) the simulation is. There is a residual for each flow variable, and the lower the residual, the more converged the flow solution is.



As would be expected (note the logarithmic y axis), the residuals drop very quickly in the first couple of hundred iterations as the flow quickly develops from the initial condition (which in this case, is the freestream condition everywhere). After that, the flow residuals (ρ , $\rho V[0]$, $\rho V[1]$, $\rho V[2]$ and ρE) residuals continue to drop, while the turbulence residuals (ρk and $\rho \Omega$) drop initially before flatlining / increasing.

This behaviour is common - the turbulence equations can take a while to react to changes in the flow field, and the initial guess for the turbulence equations is often poorer than the initial conditions for the flow field. A combination of the fact that the flow residuals have dropped several orders of magnitude over the simulation history and the fact that the residuals are in effect flat from 20,000 cycles onwards mean we can be confident that the simulation is sufficiently converged.

Plotting forces

Next, we can use the Jupyter notebook to plot the variation of the force coefficients on the aerofoil surface with cycle number.

```
r.plot_forces()
```

Check the `wall_Fx` and `wall_Fz` tickboxes - given this is a symmetrical aerofoil run at 0 angle of attack, the x force corresponds to drag and the z force corresponds to lift. We would expect zero lift and a non-zero, positive drag.

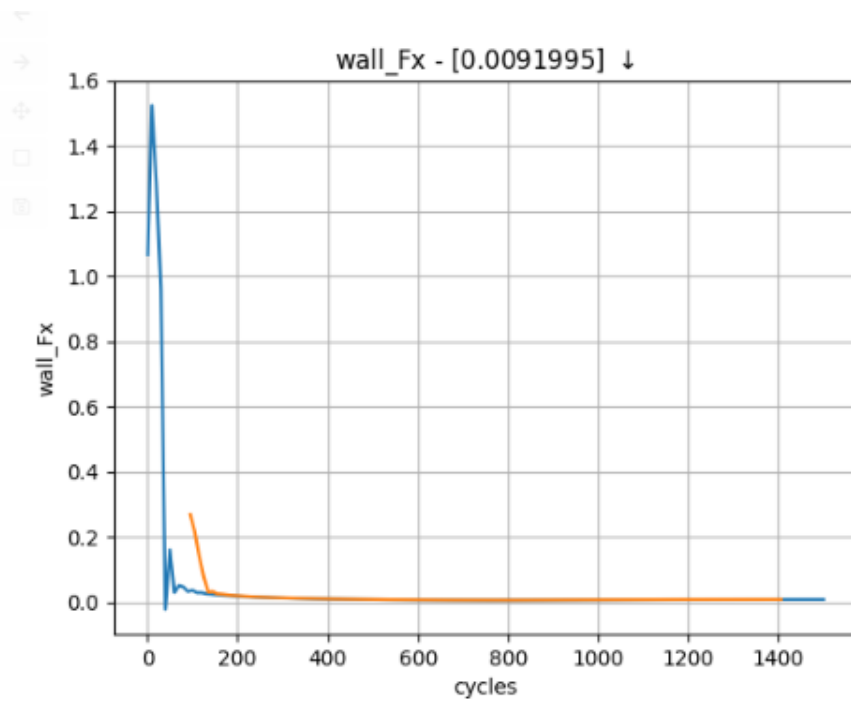
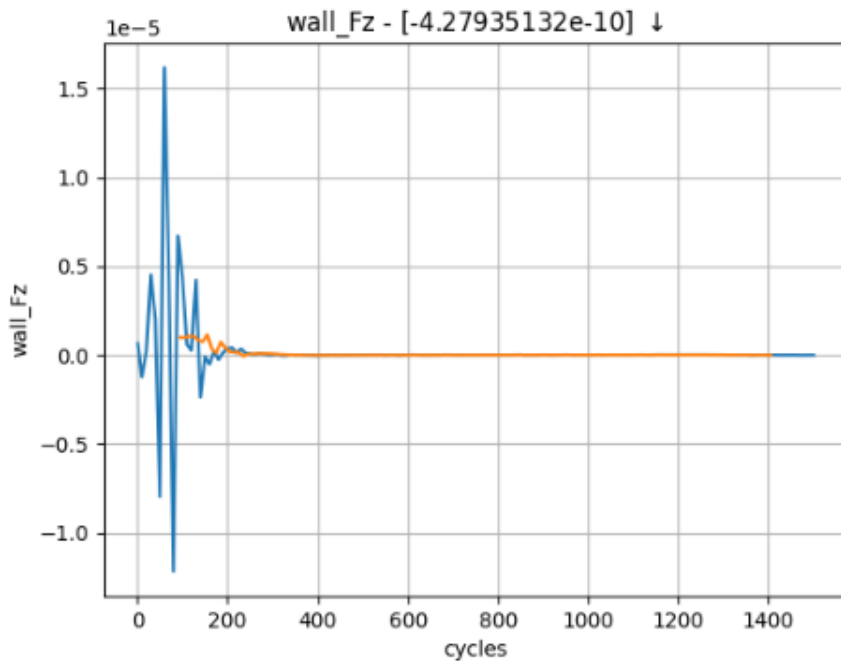


Figure 6



- | | | |
|---|-----------------------------------|---|
| <input checked="" type="checkbox"/> wall_Fx | <input type="checkbox"/> wall_Fy | <input checked="" type="checkbox"/> wall_Fz |
| <input type="checkbox"/> wall_Fpx | <input type="checkbox"/> wall_Fpy | <input type="checkbox"/> wall_Fpz |
| <input type="checkbox"/> wall_Ffx | <input type="checkbox"/> wall_Ffy | <input type="checkbox"/> wall_Ffz |

The force plots tell a similar story to the residuals - there are initially large oscillations as the flow settles down, before the force traces essentially flatline from 1200 cycles onwards.

Plotting performance

```
r.plot_performance()
```

Finally, we can plot the time used per cycle using the `plot_performance()` method. The last cycle is particularly long because it is the only cycle where the flow solution is written to a file. If an implicit solver is used, `plot_performance()` will also attempt to plot the memory usage per cycle.

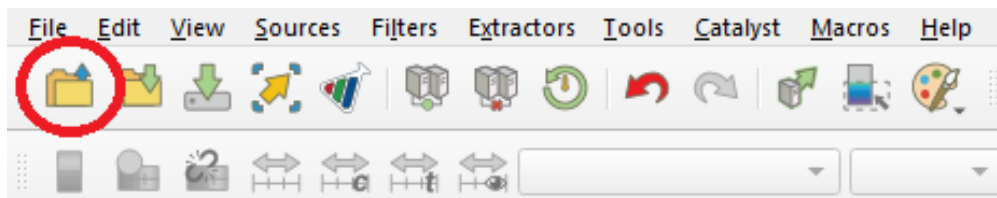
Step 6. Looking at results with Paraview

Paraview is a generally purpose visualisation tool that is the recommended way of post processing zCFD results. Please see ParaView.org for download and installation instructions.

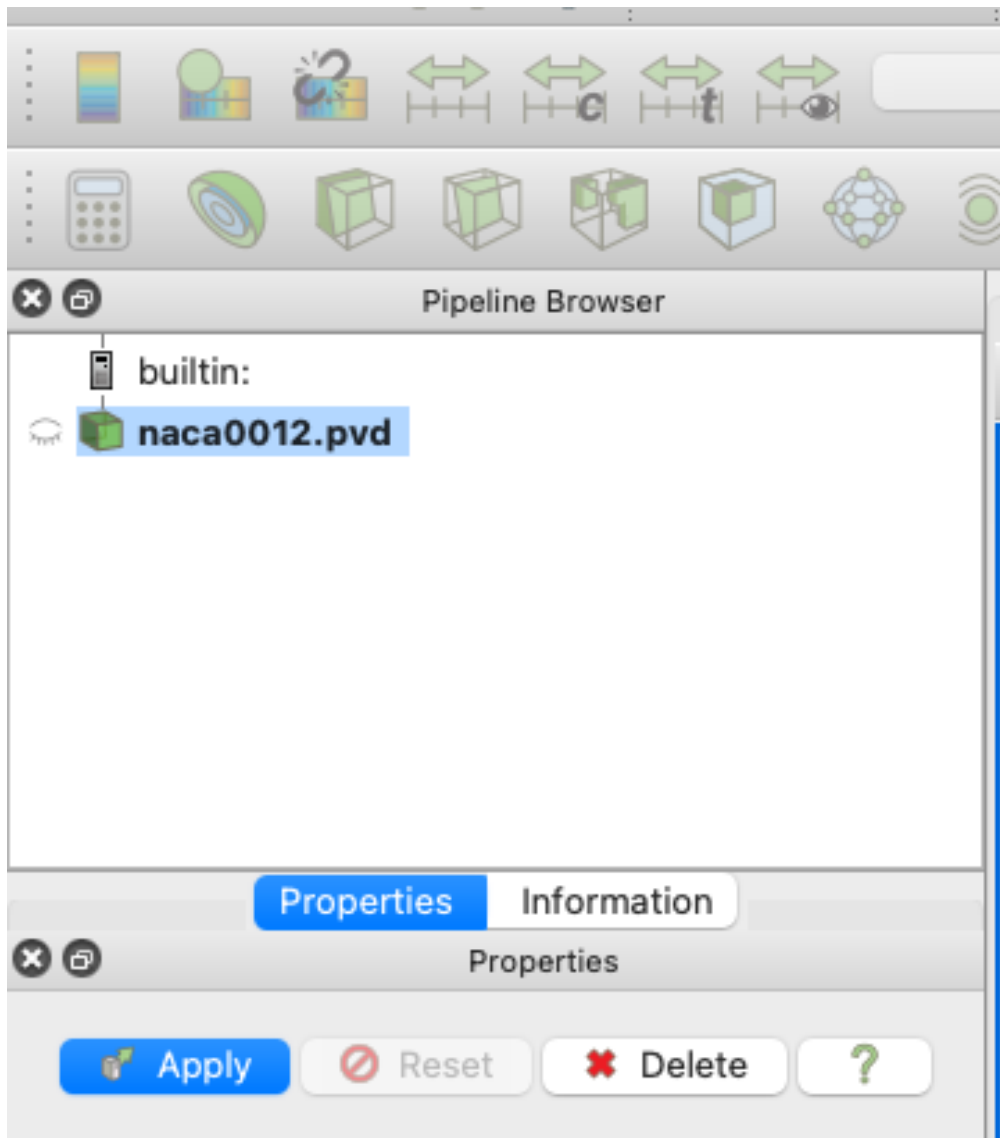
Loading your data

As mentioned above a “naca0012_P1_OUTPUT” folder has been generated, and contains a “.pvd” file (naca0012.pvd). This file can be seen as an index of all the different output files, this way, your output data is imported onto Paraview using a single file, making it easier to handle.

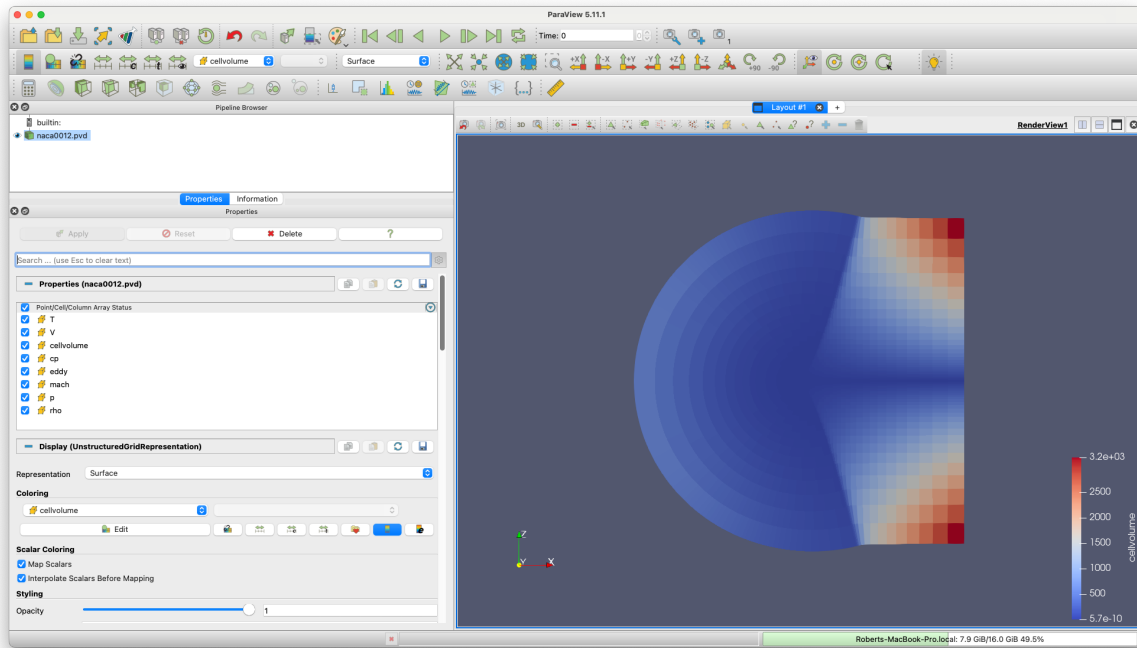
After opening Paraview, simply click on the “Open” icon shown below or go into File>Open or press Ctrl+O. Locate the directory in which you have stored your data and open naca0012.pvd.



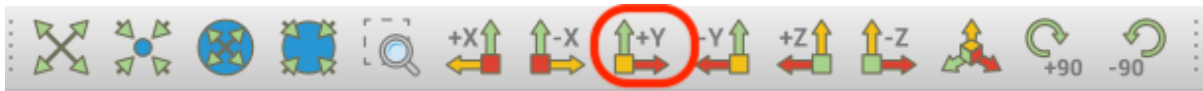
Once the file is correctly loaded in Paraview, the “Pipeline Browser” on the left of your screen should look like this:



Now you need to click “Apply”, which will lead to the following layout:



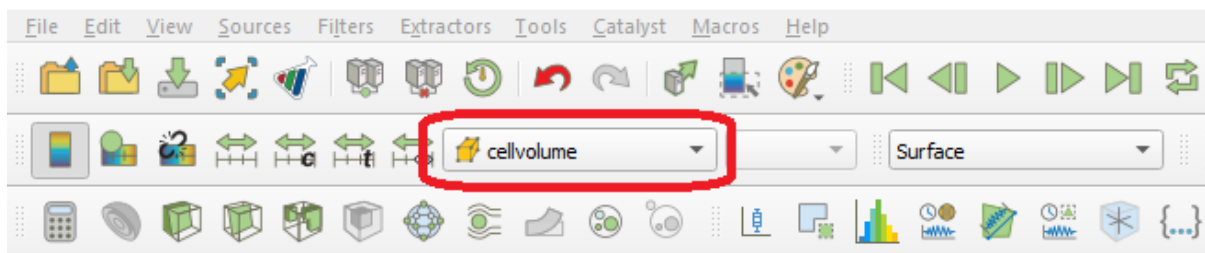
You may need to use the ‘set view direction to +ve y’ button:



Visualising Variables

By default, Paraview shows the “cellvolume” variable. This allows to see that the mesh is refined near the center of the mesh, where the airfoil is. This is common practice, as capturing the flow around a body is more demanding than doing so in the free-stream. Naturally, having a really fine mesh over the entire fluid domain would make the problem really computationally expensive.

Other variables can be selected and shown using the following scrolling menu:

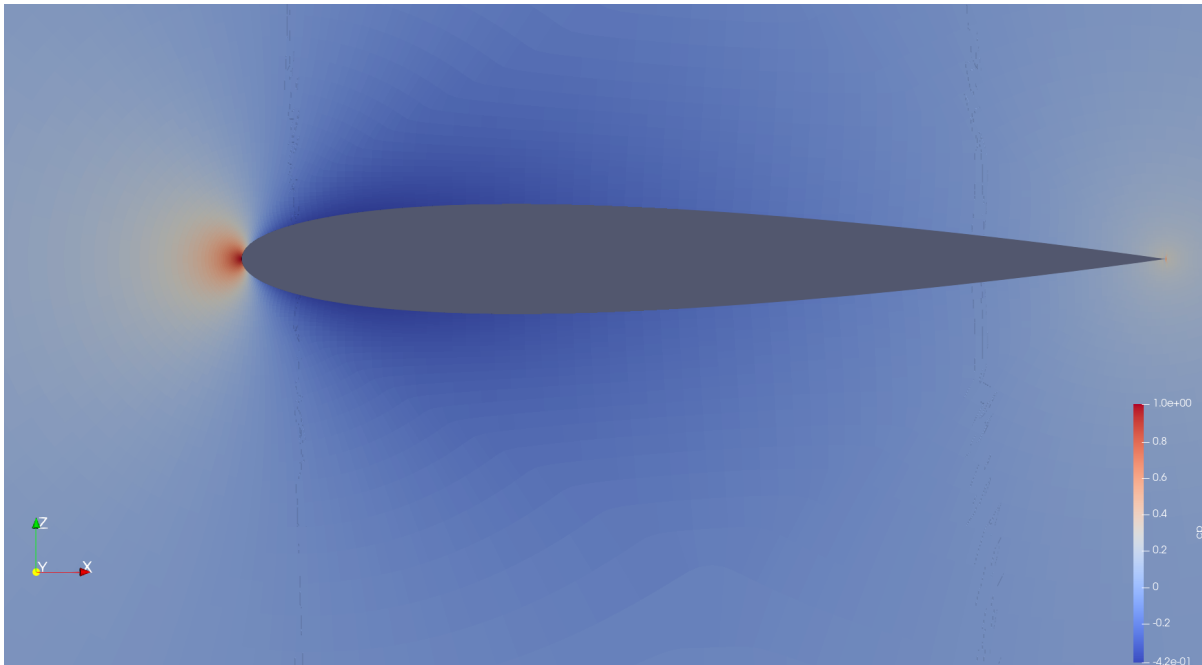


Let’s observe the pressure coefficient around the airfoil. To do so, use the scrolling menu and select the “cp” variable.

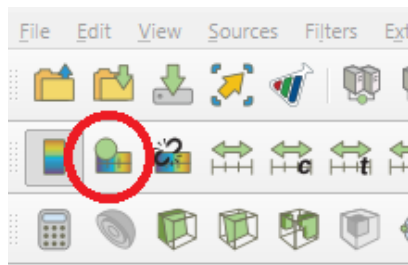
Note

The pressure coefficient is given by the following formula $C_p = \frac{p - p_\infty}{\frac{1}{2} \rho_\infty V_\infty^2}$

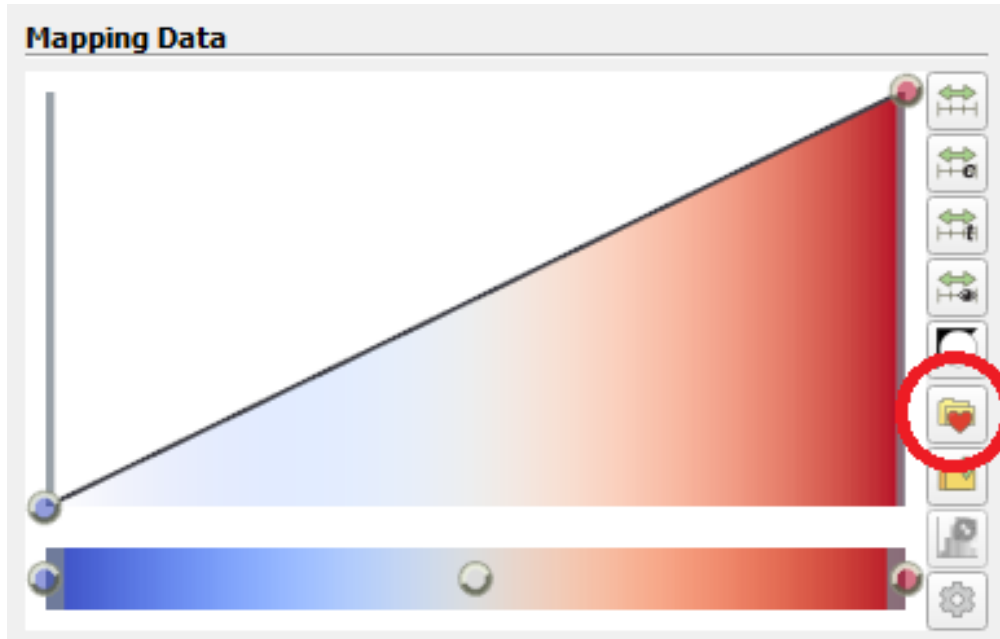
This gives the following (you will need to zoom in substantially to the centre of the mesh before you can clearly see the airfoil):



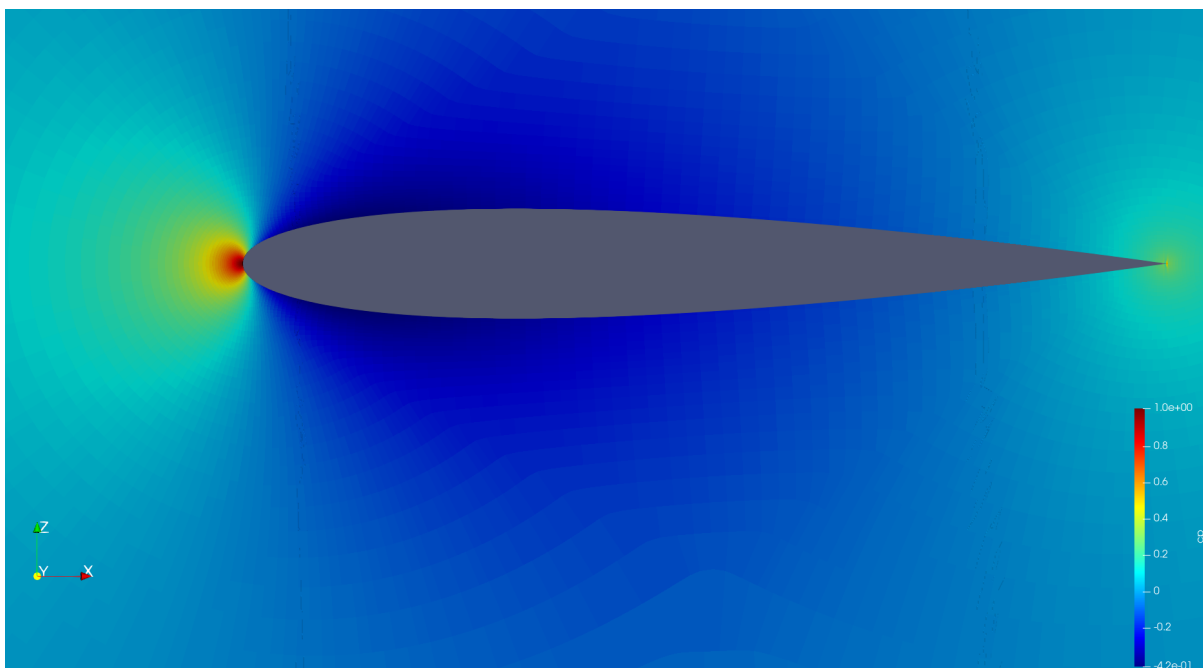
Note that you can change the colormap used by Paraview by clicking on the “Edit Color Map” icon:

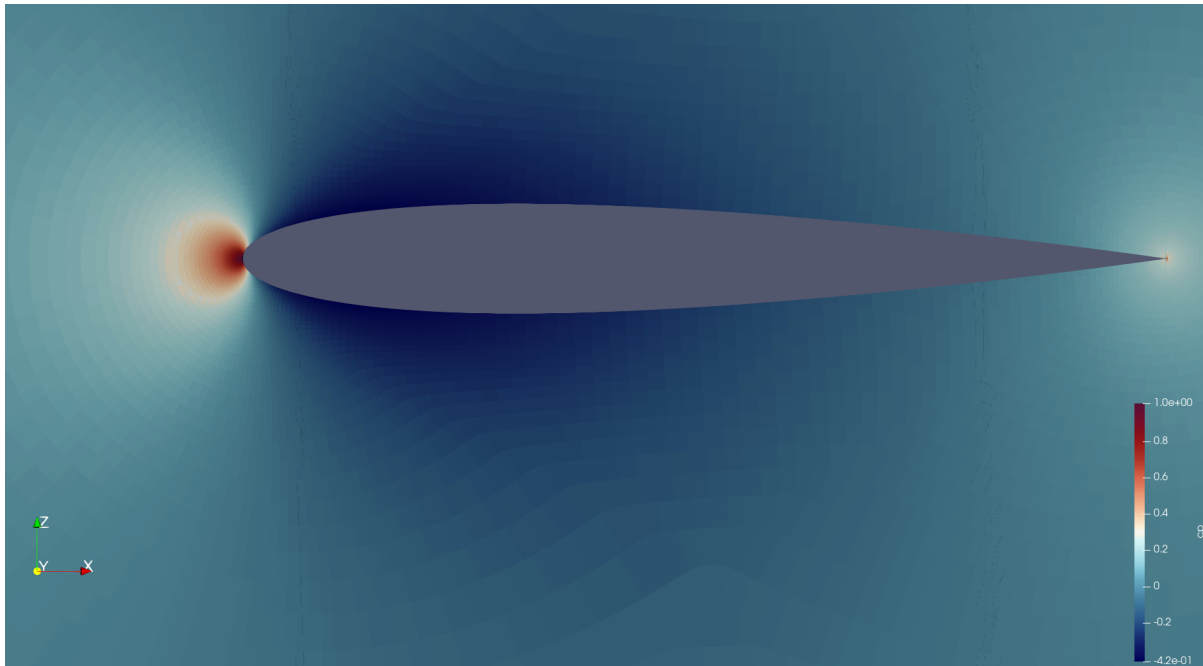


and then the “Choose Preset” icon:



Here are the same results shown using different colormaps:

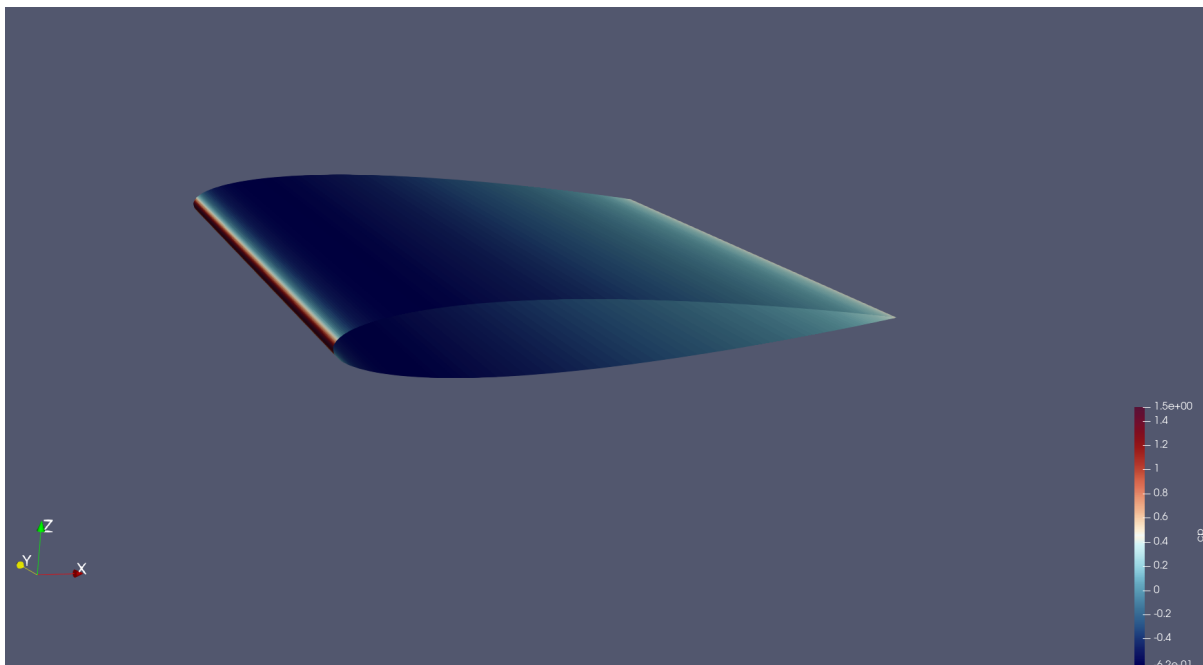




Those simple steps allow to qualitatively inspect the solution given by our CFD simulation. More advanced analysis is also feasible. A common result in aerodynamics, especially around an airfoil, is the plot of the pressure coefficient along the chord.

Pressure Coefficient Plot

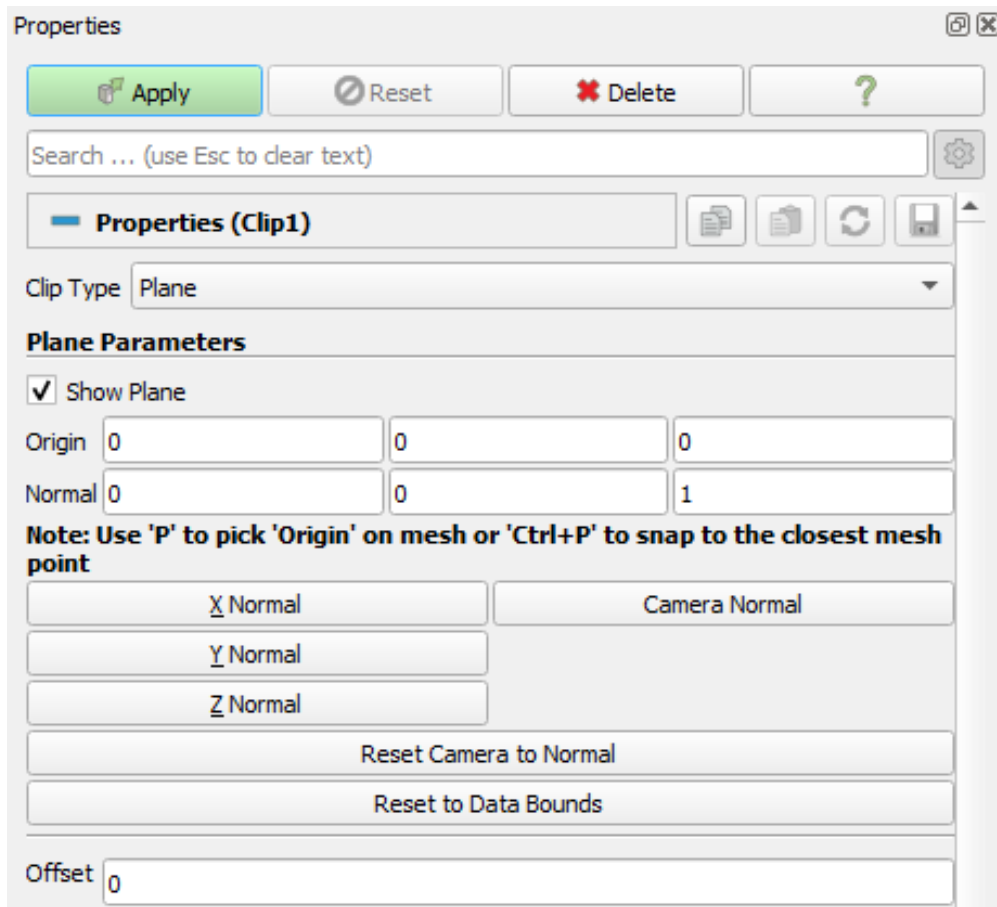
Open the “naca0012_wall.pvd” file . Naturally, the resulting image looks different from the previous as this only contains the zones where a “wall” boundary condition has been defined, which in this case happens to just be the airfoil itself.



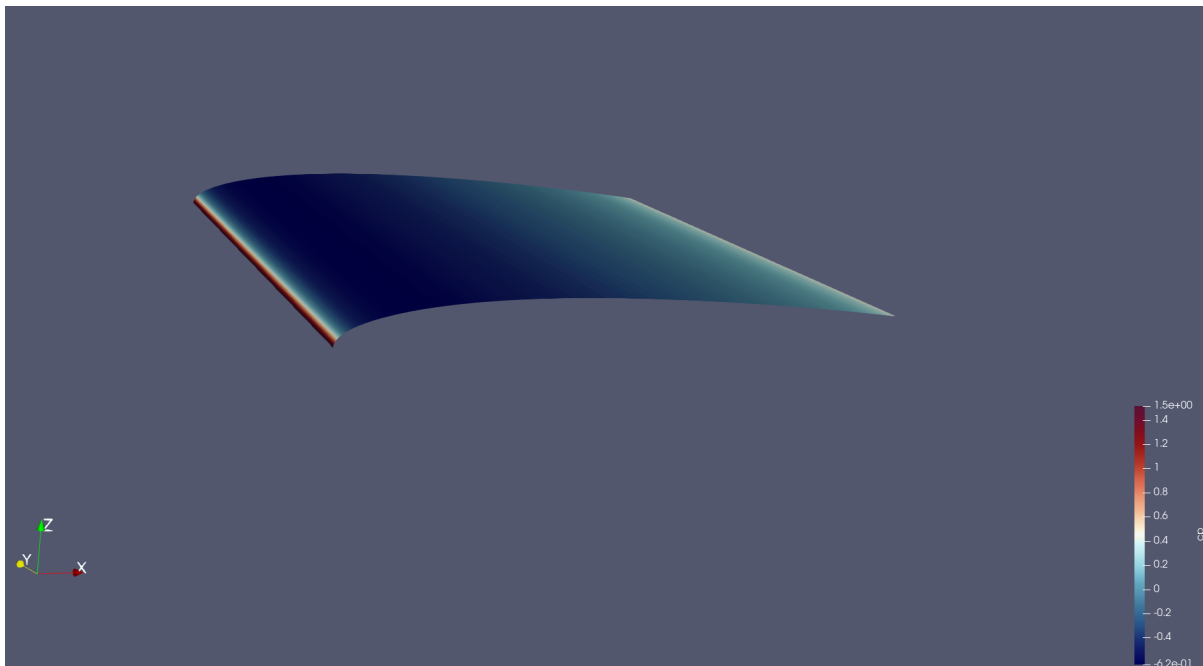
It is usually of interest to have a plot showing the pressure coefficient on the upper and the lower surface, therefore it is necessary to extract the data separately for each face of the airfoil. The upper and lower surfaces of the airfoil then need to be separated.

To this end, the “Clip” filter has to be used. To use it, right-click on the “naca0012_wall.pvd” object in the Pipeline Browser, select Add Filter -> Alphabetical -> Clip. The properties of the “Clip” filter are displayed on

the left. Firstly, untick the “Invert” option and then you should set them to the following combination:



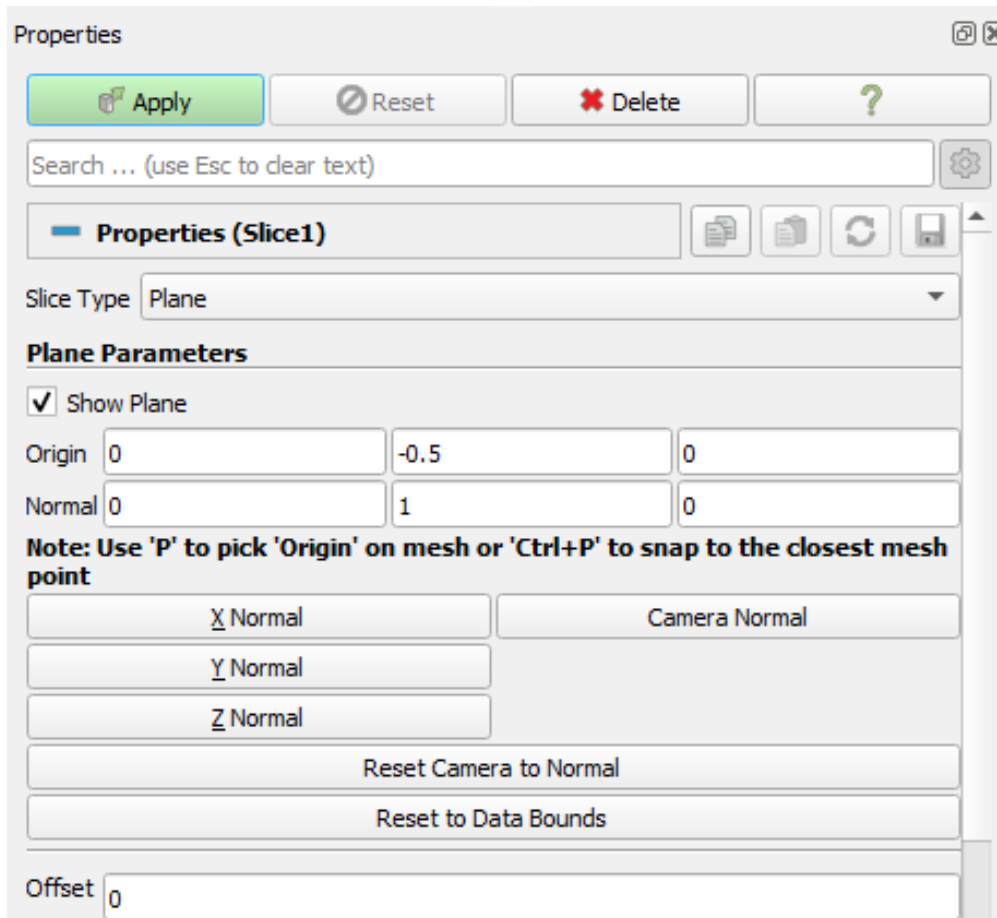
By default, this will “remove” the lower surface of the airfoil, leaving the following shape:



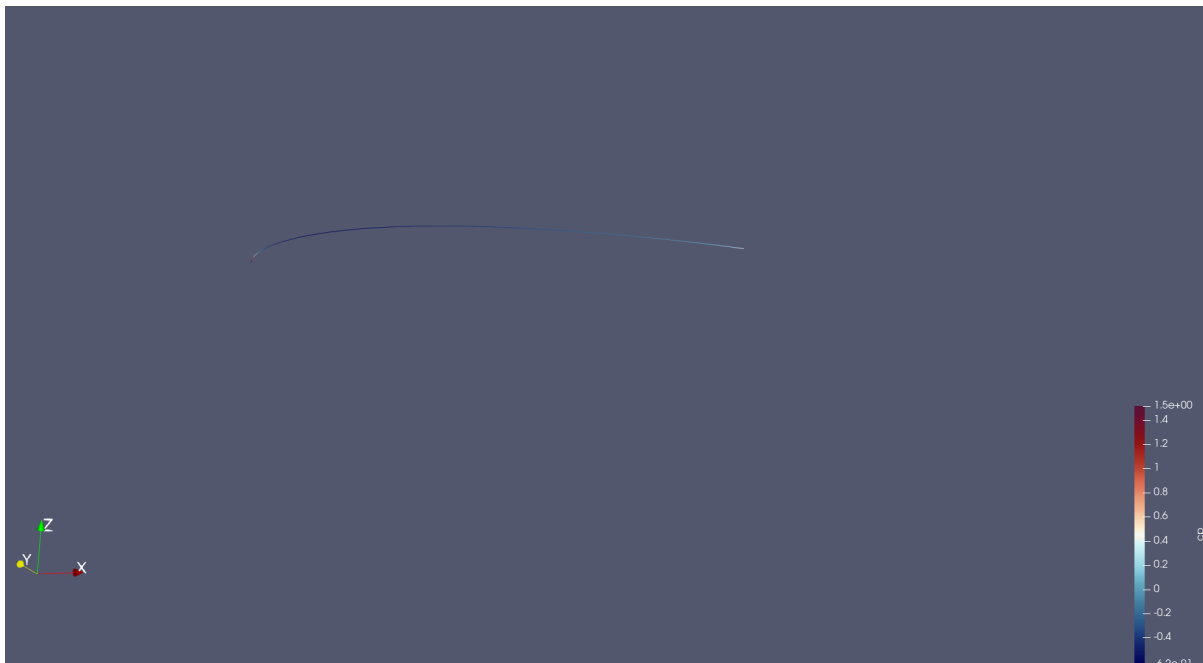
Note

To remove the upper surface instead, just tick the “Invert” option in the “Clip” filter’s properties.

Now, we want to take a “Slice” of the remaining surface. To do so, follow the same procedure as for the “Clip” filter but select the “Slice” filter instead. When prompted, set the properties of the filter to be as follows:



You should end up with this:



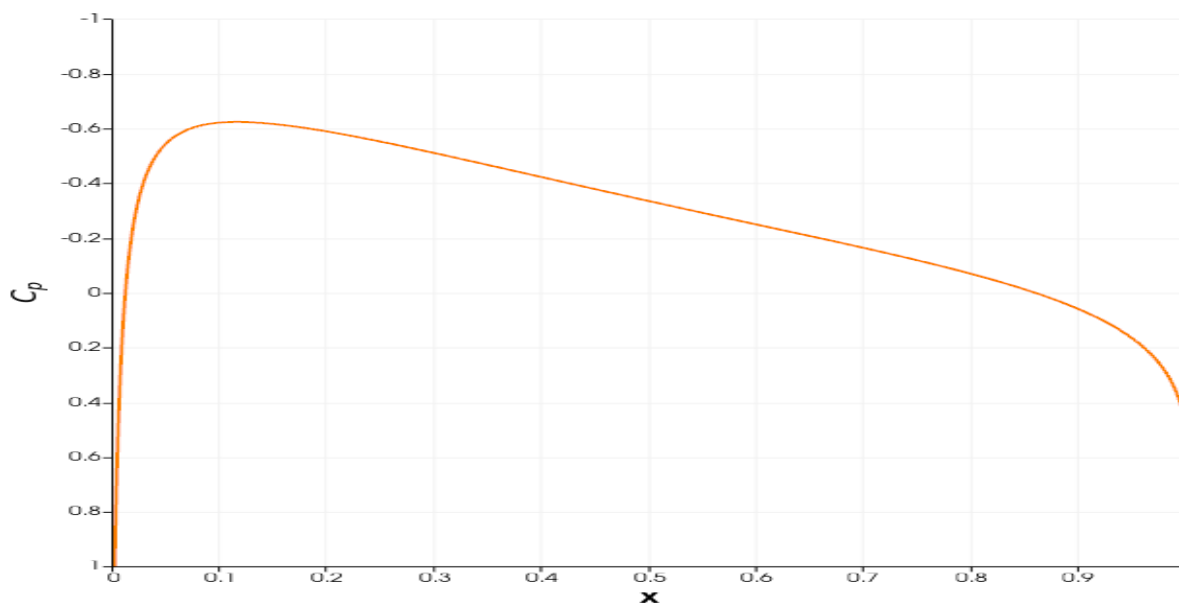
Then the data should be converted from “cell data” to “point data”. This is done by using the “CellDataToPointData” filter. Access by right-clicking on the “Slice” object selecting “Add filters”.

Once this is done, a plot can be produced in Paraview using the “PlotOnSortedLines” filter. Right-click on

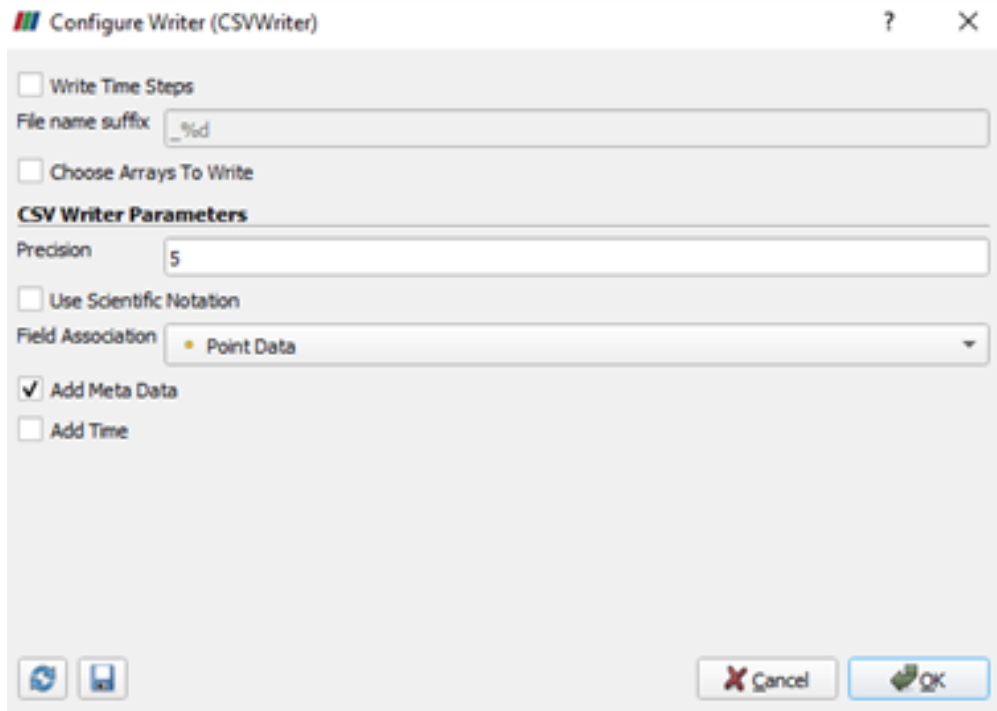
the “CellDatatoPointData1” object created previously and add the “PlotOnSortedLines” filter. A plot should appear on the right. You can select the variables to plot in the “Properties -> Series Parameters” window, as well as changing the settings of the axis. Select the “cp” variable in “Series Parameters”, and use ‘Points_X’ as the ‘X Array Name’. Untick ‘Show Legend’, set ‘Left Axis Title’ to ‘\$C_p\$’ and set the ‘Bottom Axis Title’ to ‘x’. You can also use the “Left Axis Use Custom Range” option to change the y-axis range:

Left Axis	
Left Axis Title	<input type="text" value="\$C_p\$"/>
Left Axis Range	
<input type="checkbox"/> Left Axis Log Scale	
<input checked="" type="checkbox"/> Left Axis Use Custom Range	
Left Axis Range Minimum	<input type="text" value="1"/>
Left Axis Range Maximum	<input type="text" value="-1"/>
Bottom Axis	
Bottom Axis Title	<input type="text" value="x"/>

Note that setting the maximum as a negative number will “invert” the y-axis and the negative numbers will be shown “at the top”.



The data can be exported as a .csv file, which can then be manipulated in Python, Excel, MATLAB or any other software. To do so, go to File -> Save data -> *select a folder and give a name to the file*. The following window should appear:



By default, Paraview writes all the variables into the .csv file. However, if only a few of them are of interest, you can use the “Choose Arrays To Write” option.

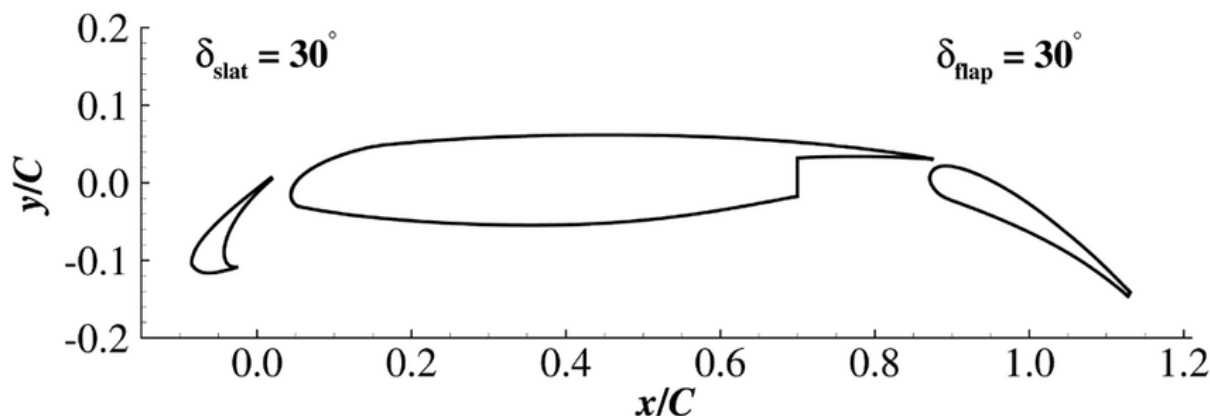
Now, this procedure can be repeated for the lower surface of the airfoil. A pressure coefficient plot can then be made for validation purposes.

1.4.2 Tutorial 2: Steady State RANS

Table of Contents

- *Control Dictionary Breakdown*
- *Running the case*
- *Monitoring convergence*
- *Plotting force convergence*
- *Paraview*
- *Citations*

In Tutorial 1, we learnt how to run a case in zCFD and visualise the results. We will now use a more complex test case to showcase some of the features of the solver. The case we will look at is the 30P30N aerofoil, which is a 2D multi element aerofoil, developed as an acoustic benchmark case [1]. The geometry of this case can be seen below:



Initially we will begin by obtaining a steady state RANS solution.

The required meshes and control dictionary can be found [here](#). The case has 64,000 cells, and will run in less than 10 minutes on an NVIDIA RTX 3060 GPU.

This case is run as a steady state simulation, using an implicit time marching scheme. The Reynolds Averaged Navier-Stokes equations are solved using Menter's SST turbulence model with wall functions.

Control Dictionary Breakdown

The setup for this case is very similar to the previous NACA0012 cases, but the control dictionary does feature some extra terms which can be useful for a more streamlined workflow.

Reference variables

At the top of the control file, the key variables for the case- Reynolds number, Mach number, temperature etc... are all hard coded, and then referred to later in the script. In cases where you might want to run many simulations with slightly different values to change, this can be an effective way to ensure consistency with variables. Additionally this allows implicit values such as the reference velocity, and freestream Mach to be calculated automatically in the script.

```
# create variables to assign main experimental parameters
reynolds = 1.71e6
mach = 0.17
T = 295.56
p = 101325
R = 287.6
gamma = 1.4
reference_length = 0.457
alpha = 5.5

# calculate implicit values
rho = p / (R * T)
U = math.sqrt(gamma * R * T) * mach

# assign each mesh zone to a boundary
wall = [6]
symmetry = [4,5]
farfield = [7]
```

Scale

In this case a scaling is applied to convert the size of the mesh. The .h5 mesh file was generated with units of inches, whereas the flow conditions are specified in SI units, therefore a scaling of 0.0254 is applied to convert the mesh into metres. The z (spanwise) direction has been scaled to be 1 metre wide. The mesh has only a

single cell in the z direction so no spanwise flow is expected - making the z extent of the mesh 1 metre simply means that the forces and moments reported by zCFD will already be per unit span.

```
# scale the mesh to match the experimental data
'scale' : [0.0254,0.0254,0.0254/0.127],
```

Inflow vector

In this case we want to simulate the aerofoil operating at an angle of attack of 4 degrees. Rather than rotating the mesh, it is easier to rotate the inflow vector relative to the mesh, an example of a Galilean transformation. The `zutil` function `vector_from_angle()` calculates the inflow vector given an x-z angle of attack, x-y angle of attack and flow speed.

```
'IC_1' : {
  'temperature': T,
  'pressure': p,
  'V': {
    # calculate the inflow vector based on the angle of attack
    'vector' : zutil.vector_from_angle(0.0,alpha,U),
  },
  'Reynolds No' : reynolds,
  'Reference Length' : reference_length,
  'turbulence intensity': 0.01,
  'eddy viscosity ratio': 0.1,
  'ambient turbulence intensity': 1e-20,
  'ambient eddy viscosity ratio': 1e-20,
},
```

Transform

The lift and drag forces acting on a body are defined relative to the freestream flow, lift normal and drag parallel. In this case, where we have rotated the relative inflow vector to a specific angle of attack, it is also useful to rotate the force report by the same vector. The transformed forces will appear as `Ft_` terms in the report file.

```
# define a function to rotate the output forces by the angle of attack
def my_transform(x,y,z):
  v = [x,y,z]
  v = zutil.rotate_vector(v,0.0,alpha)
  return {'v1' : v[0], 'v2' : v[1], 'v3' : v[2]}
```

Running the case

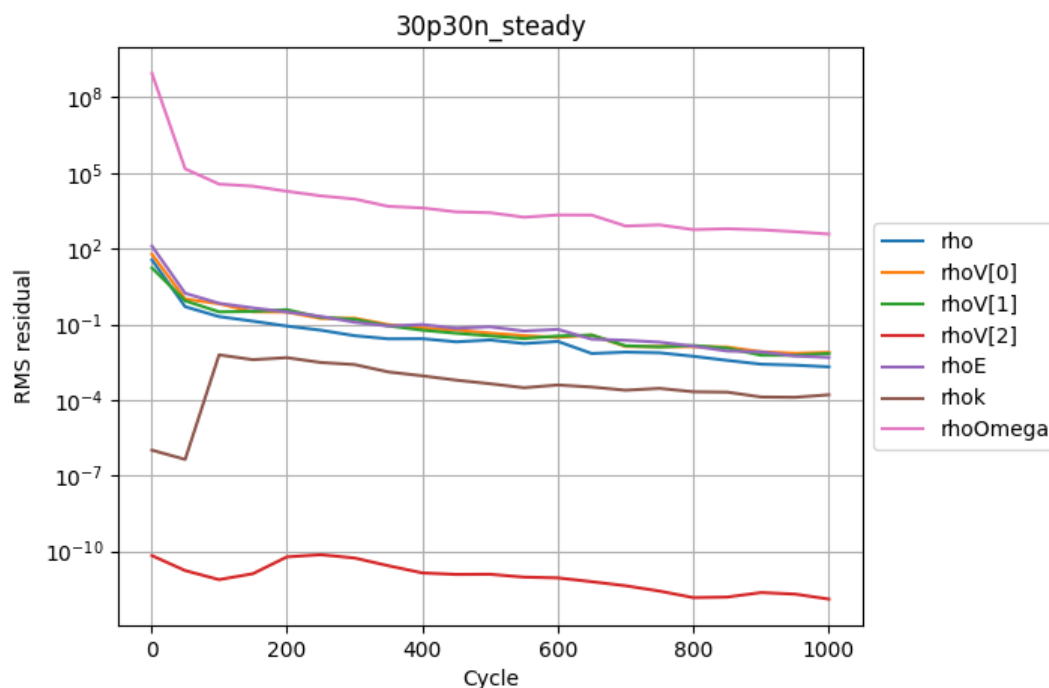
You can run the case as you did for Tutorial 1, but with the following `run_zcfd` command:

```
run_zcfd -m 30p30n_coarse.h5 -c 30p30n_steady.py
```

Monitoring convergence

Start by launching a Jupyter server to examine the residuals in the `30p30n_steady_report.csv` file. Running the first cell from the `30p30n_steady_report.ipynb` notebook will plot the residuals for the continuity, momentum, and energy equations, as well as the residuals from the turbulence model.

If the case is still running you can update the plot by rerunning the cell, this provides a way to monitor the progress of a running simulation.



You will notice that case is set to run for 1000 cycles but looking at the plots, it looks like the residuals are still converging. So we will now restart the solver from where we finished and run on for another 1000 cycles.

Performing a restart

To restart the solver we need to update the `'restart'` parameter in the control dictionary. If this is set to `False` the solver will always perform a fresh start, if it is `True` then a results file will be read in and the solve will start based on the data in that file. To enable the restart edit `30p30n_steady.py` and change `restart` to `True`. You will also need to update `'cycles'` to 2000.

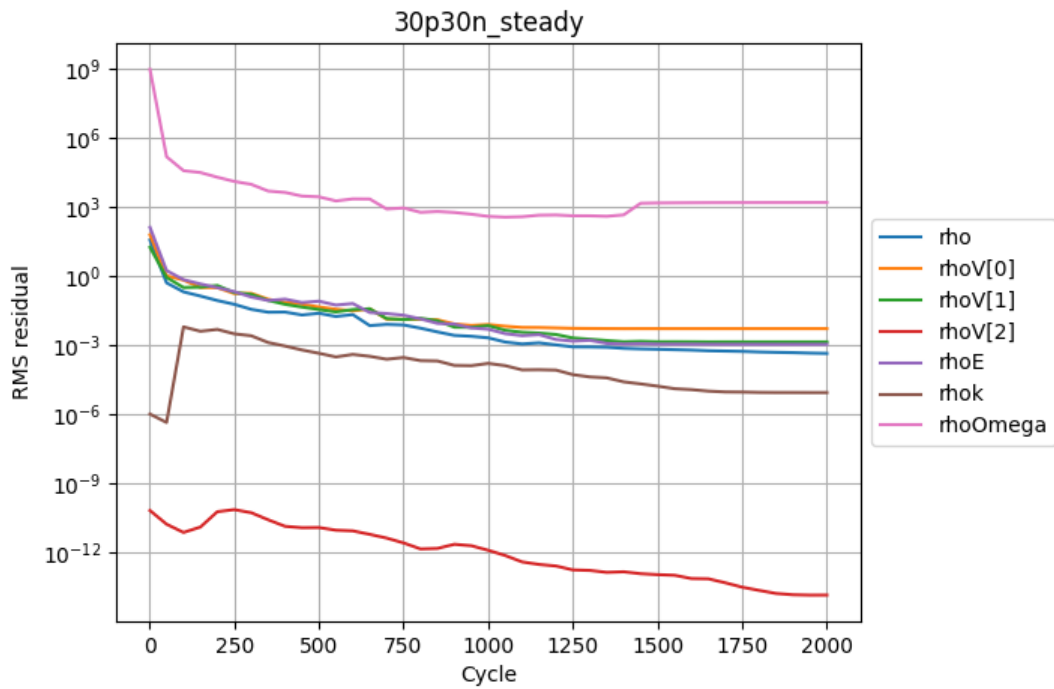
```
"restart": True,

'time marching' : {
    ...
    'cycles' : 2000,
    ...
}
```

By default zCFD will look for a results file with the same name as the current case file, appended with `'_results.h5'`. So in our case it will look for `"30p30n_steady_results.h5"`. When you have edited the control dictionary go ahead and restart the simulation again using the same `run_zcfd` command:

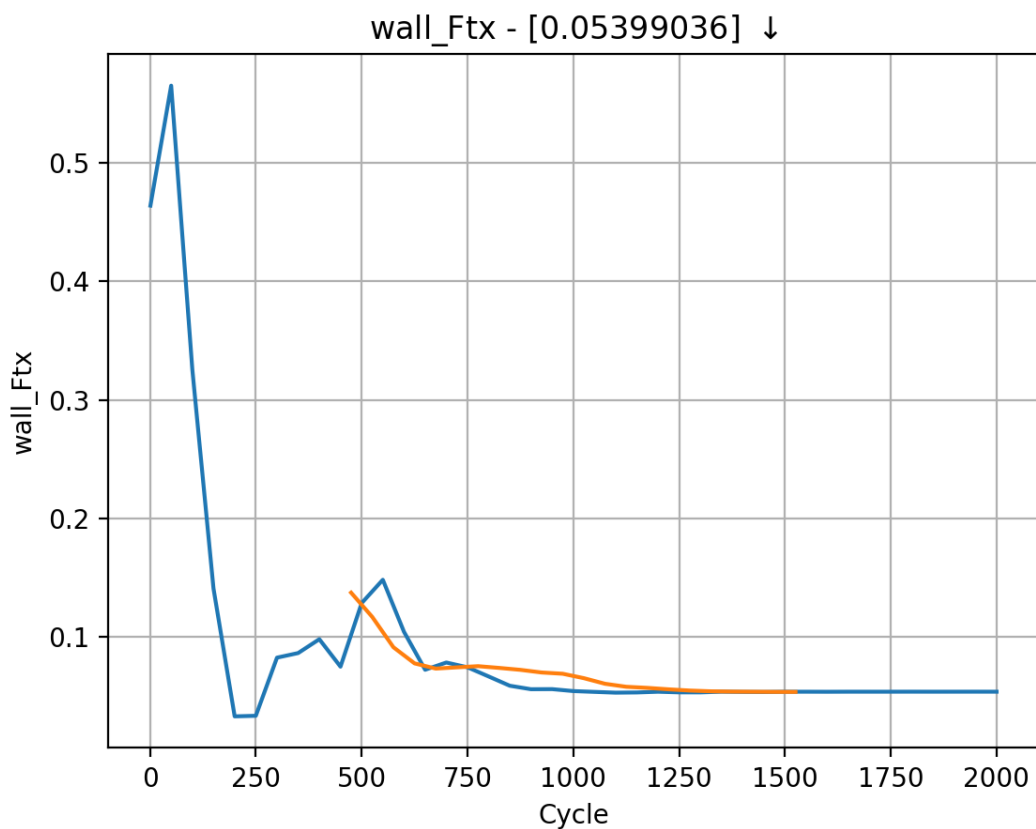
```
run_zcfd -m 30p30n_coarse.h5 -c 30p30n_steady.py
```

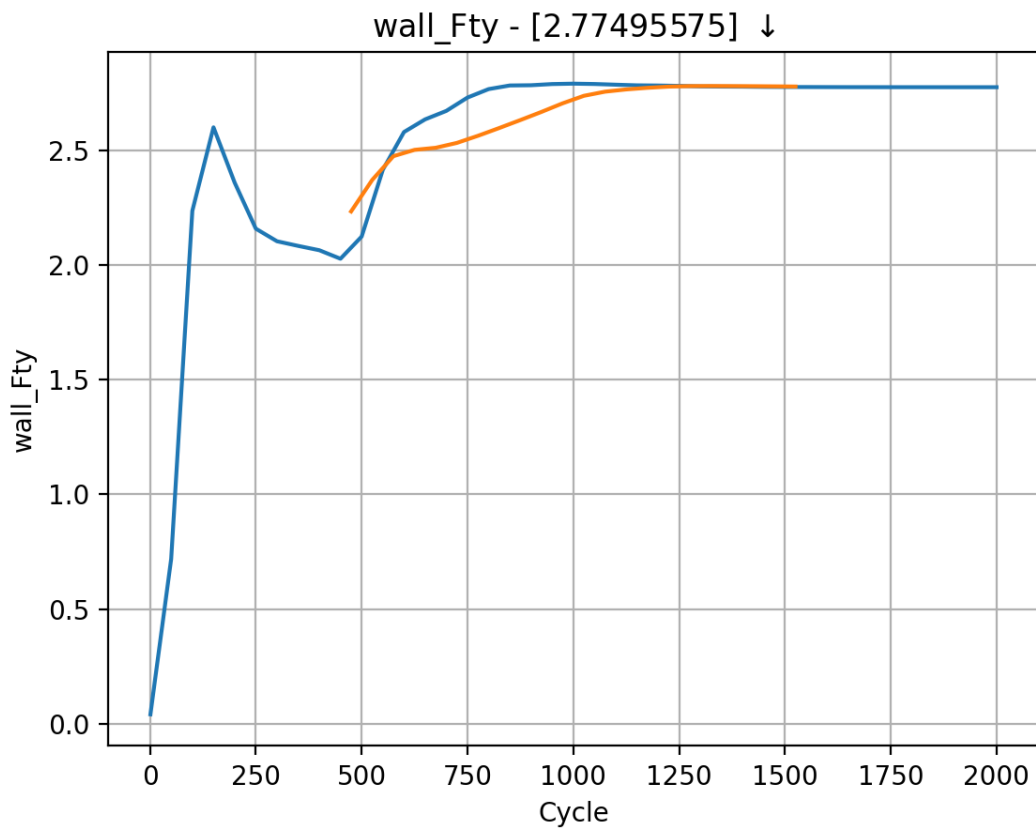
Once the solver has finished rerun the cell in the notebook to examine the residuals again. The residuals now look like they have converged:



Plotting force convergence

Examining the force convergence history next, we are interested in the x and y forces, but transformed by the inflow vector, therefore the wall_Ftx and wall_Fty plots are of interest.

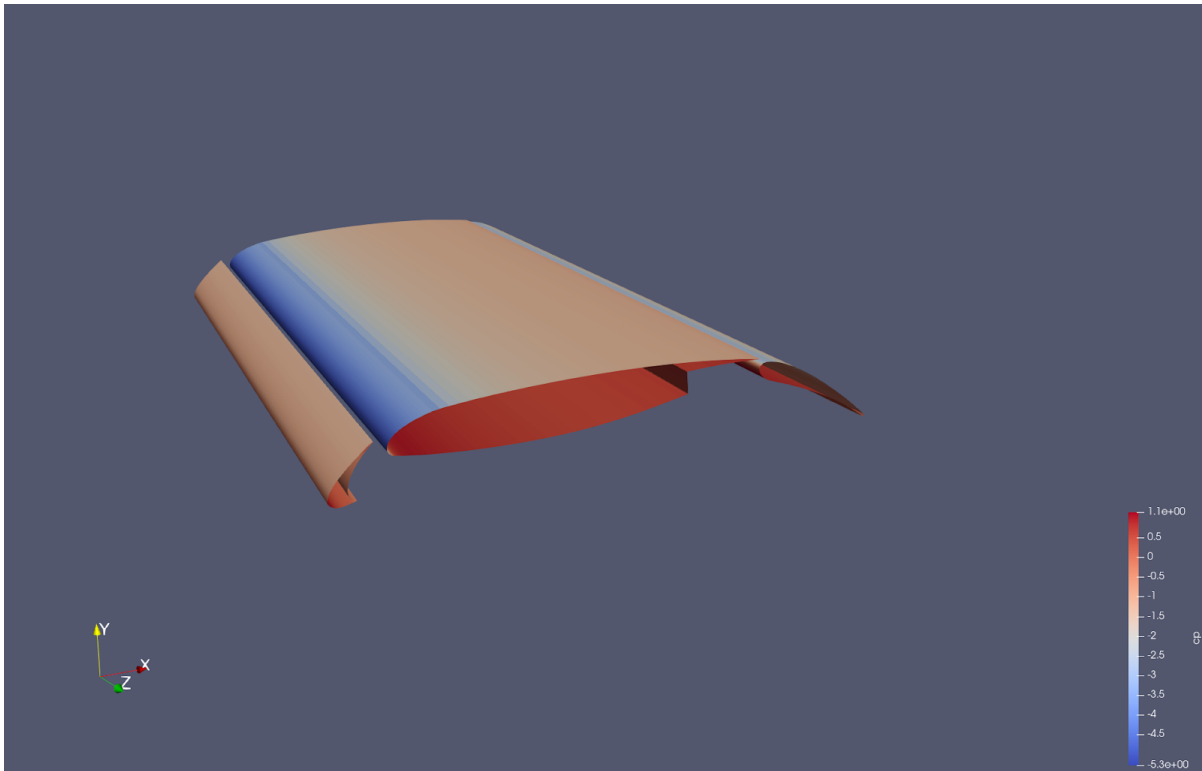




Which show reasonable agreement with experimental results, and additionally that the forces are at least nearing convergence. The grid for this case is still extremely coarse, accounting for the differences in lift and drag coefficients.

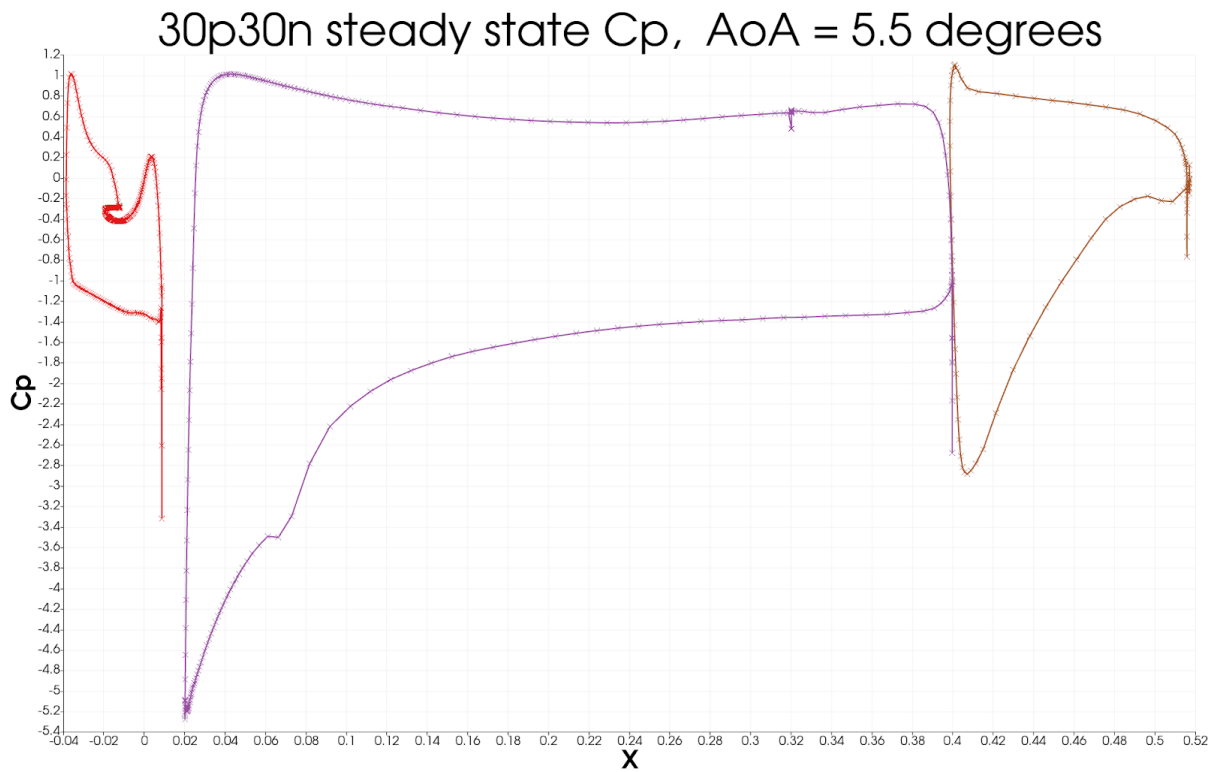
Paraview

Opening Paraview, and loading in the *30p30n_steady_wall.pvd* results will allow you to view the aerofoil surface results:



To get a continuous plot of c_p against x/c you need to use a plot over sorted lines filter. To do this:

1. On the surface data apply a *'cell data to point data'* filter.
2. On the *cell data to point data* apply a *'slice'* filter, ensuring the slice uses a z normal, and is centred through the middle of the airfoil
3. On the *slice* data apply a *'plot on sorted lines'* filter and click apply. This will then bring up a new *'line graph'* view.
4. Make sure to select all 3 segments in the composite data set dialogue box, then ensure only the c_p variables are selected in the series parameters. Finally for the X Array name, select *'Points_X'*
5. Modify the style and markers until you are happy with the result.



Citations

1. Zhang, Yufei & Chen, Haixin & Wang, Kan & Wang, Meng. (2017). Aeroacoustic Prediction of a Multi-Element Airfoil Using Wall-Modeled Large-Eddy Simulation. AIAA Journal. 55. 1-15. 10.2514/1.J055853.

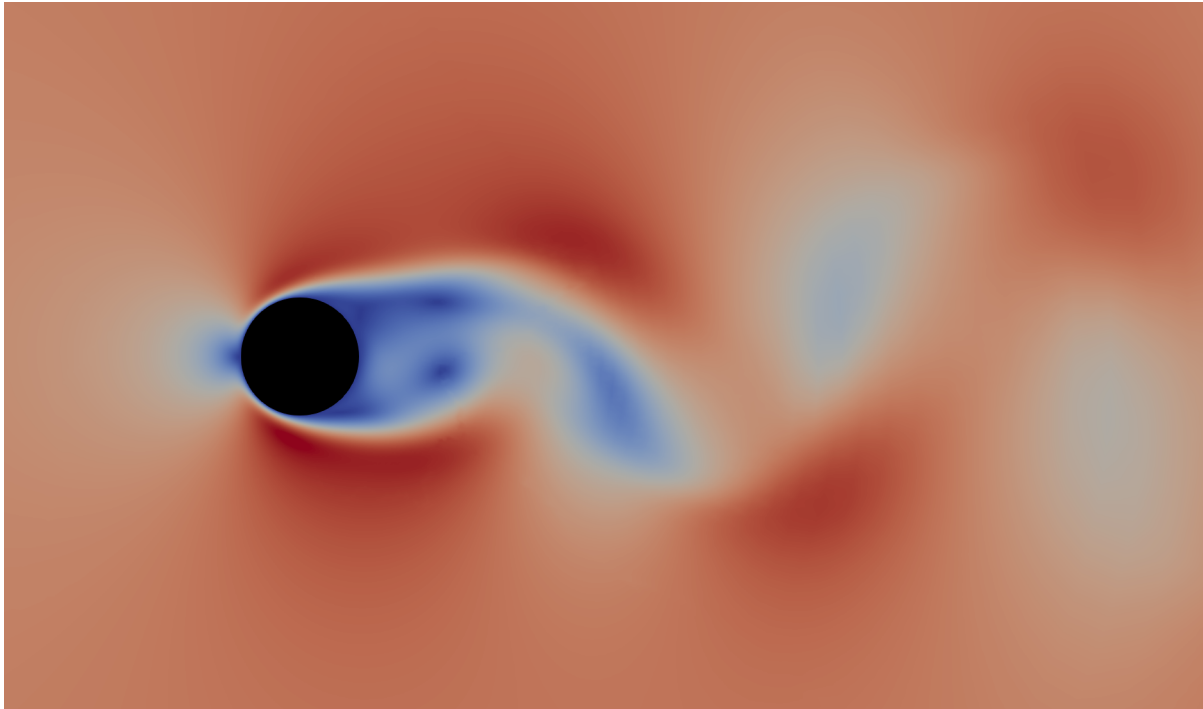
1.4.3 Tutorial 3: Time accurate solution

Table of Contents

- *Introduction*
- *Control Dictionary Breakdown*
- *Running the case*
- *Post Processing*

Introduction

Following on from executing the steady state simulation of *Tutorial 2*, this tutorial will explore the generation of a time accurate result for the unsteady laminar shedding from a 2D cylinder.



You can download the required files [here](#).

Control Dictionary Breakdown

This case uses a similar control dictionary as the previous 30p30n steady state simulation, with the main difference being the time marching, and output regions of the file.

Time Marching

To switch to a time accurate simulation we need to update the “*time marching*” dictionary. In the steady state *tutorial 2* case the ‘*total time*’ and ‘*time step*’ parameters were both set to 1.0, this causes the solver to run a single steady state timestep for the number of cycles defined by the ‘*cycles*’ parameter.

We will now update these to run the time accurate simulation. To do this we set ‘*total time*’ to be 1.2, which means the simulation will be run for a total of 1.2 seconds. ‘*time step*’ is set to 0.002 seconds, this is the interval at which the solver will step time forwards. Which means we will have a total of $1.2 / 0.002 = 600$ total unsteady timesteps to perform.

```
'time marching' : {
  'unsteady' : {
    'total time' : 1.2,
    'time step' : 0.002,
    'order' : 'second',
    'start' : 0,
  },
  'scheme' : {
    'name' : 'implicit euler',
    'stage' : 1,
  },
  'cfl': 200,
  'cfl viscous factor': 1.0E-6,
  'cfl ramp factor': {"initial": 0.1, "growth": 1.05},
  'cycles': 5,
},
```

zCFD uses dual time stepping to advance in real time by first iterating to convergence on an inner steady state ‘pseudo time’ loop, before advancing the real time cycle. In this case the inner loop is performed using

implicit euler time marching, the number of cycles this inner loop performs is controlled by *'cycles'*. So the in the example above the inner loop runs at a CFL of 200 for 5 cycles.

The choice of timestep size, and number of cycles per inner loop will have a significant effect on the quality and cost of the final solution. Using too large of a real time step will mean higher frequency unsteady effects are lost, similarly too few inner cycles will result in unsteady effects being lost. A rule of thumb is to ensure the residuals converge by at least two orders of magnitude over an inner cycle. On the other hand if too many cycles or timesteps are performed, the cost of the simulation will quickly increase. Finally the number of cycles to reach convergence in a pseudo time loop also depends on the step size. Meaning in some cases it is actually beneficial to run a smaller timestep, in order to require fewer inner loop iterations.

Output

The *'write output'* dictionary in the control dictionary is a bit more complicated here than in [tutorial 1](#) or [tutorial 2](#).

```
"write output": {
  "format": "vtk",
  "surface variables": ["V", "p", "T", "rho", "cp"],
  "volume variables": ["V", "p", "T", "rho", "m", "cp"],
  "frequency": {
    "volume data": 5,
    "surface data": 5,
    "checkpoint": 20,
  },
},
```

First of all, the *'frequency'* parameter takes on a different meaning in a time-accurate simulation ([tutorial 1](#) and [tutorial 2](#) are both steady-state simulations).

In a steady-state simulation, the *'frequency'* parameter controls how the number of pseudo-time *'cycles'* between solver outputs. Since we have no real interest in any data apart from the converged data at the end for a steady-state simulation, every time the solver outputs data, it over-writes the previous output data.

We run time-accurate simulations when we're interested in the variation of the flow over time (e.g. due to vortex shedding), so in the time-accurate solver data outputs are not over-written, and the *'frequency'* variable relates to the number of real time steps between outputs, instead of number of pseudo-time cycles between outputs.

While we can just use a single number for *'frequency'* (e.g. `"frequency": 5`), we can also specify *'frequency'* as a dictionary for more fine grained control. This is especially relevant in time-accurate simulations, where frequent data output can not only slow down the simulation but also quickly use up disk space. Generally the volume data takes longest to output, so for large cases it can be a good idea to output volume data output infrequently, and instead rely on surface data, [monitor points](#) and [volume intepolated data](#) for high frequency data collection.

In this, a relatively small case, we have chosen to output surface and volume data every 5 real time-steps. Since the *'time step'* was set to 0.002 seconds, the volume and surface data will therefore be written out every 0.01 seconds of simulated time. We have chosen to output *checkpoint* data (see [here](#)) less frequently.

Monitor Points

In order to capture the shedding frequencies of vortices behind the cylinder, we will place a monitor point in this region to append data to the report file. A monitor point will simply report the requested output variables, at the point defined within the flow. These results can be visualised alongside the force report in the output notebook.

```
"monitor": {
  "MR_1": {
    "name": "probe",
```

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```

    "point": [0.25, 1.07, 0.313],
    "variables": ["cp"]
  }
},

```

Running the case

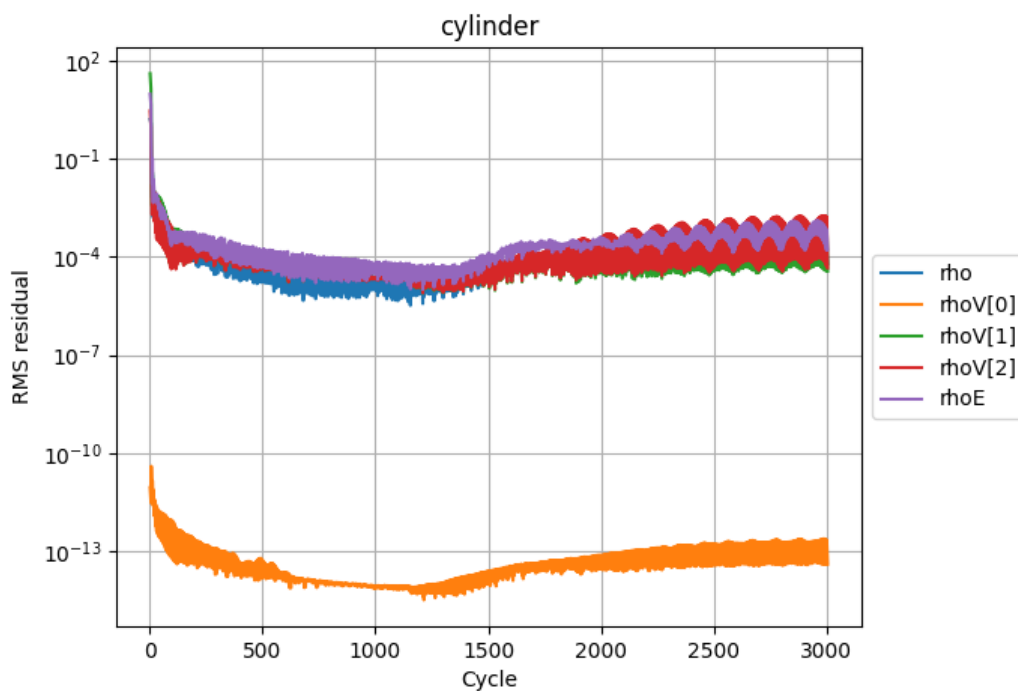
You can run the case as you did for Tutorial 1, but with the following `run_zcfd` command:

```
run_zcfd -m cylinder.h5 -c cylinder.py
```

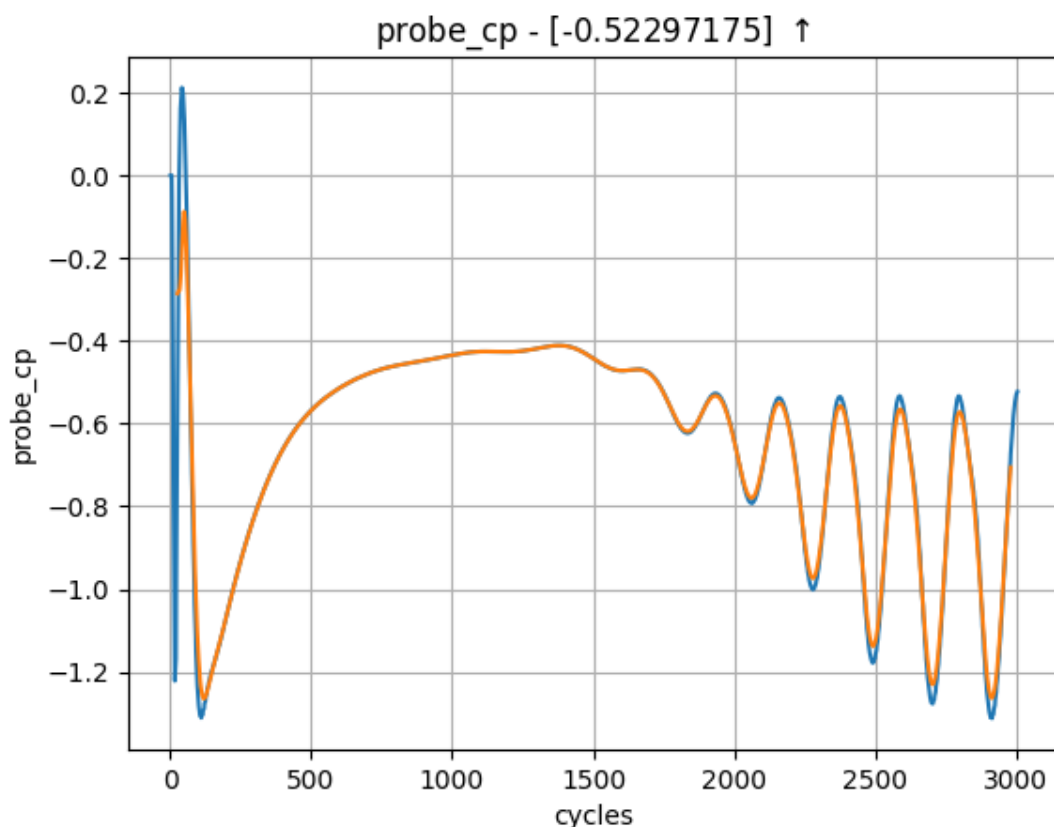
Post Processing

Output report

Start and connect to a Jupyter server, using `'start_lab'` as outlined in the previous sections. Go ahead and run all cells.



In the `"plot_forces"` cell, you should notice additional data points available provided by the monitor point. Visualising the pressure trace [`probe_cp`] should reveal an oscillatory pattern, indicating that the predicted vortex shedding is indeed occurring. This trace can then be used to calculate the corresponding shedding frequency.

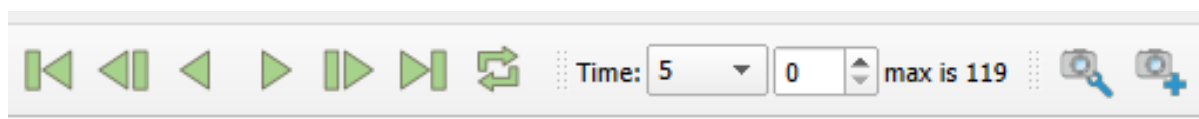


Flow field

We set the output frequency to 5 when running the case and so the solver will have written visualisation VTK files every 5 real time steps. If you look in the `'cylinder_P1_OUTPUT/VISUALISATION'` directory you will see a series of `.vtp` and `.pvtpp` files, one for every written timestep.

You could load these individually but the easier method is to load the `'cylinder.pvd'` in `'cylinder_P1_OUTPUT'`. This `.pvd` file links to all of the timesteps.

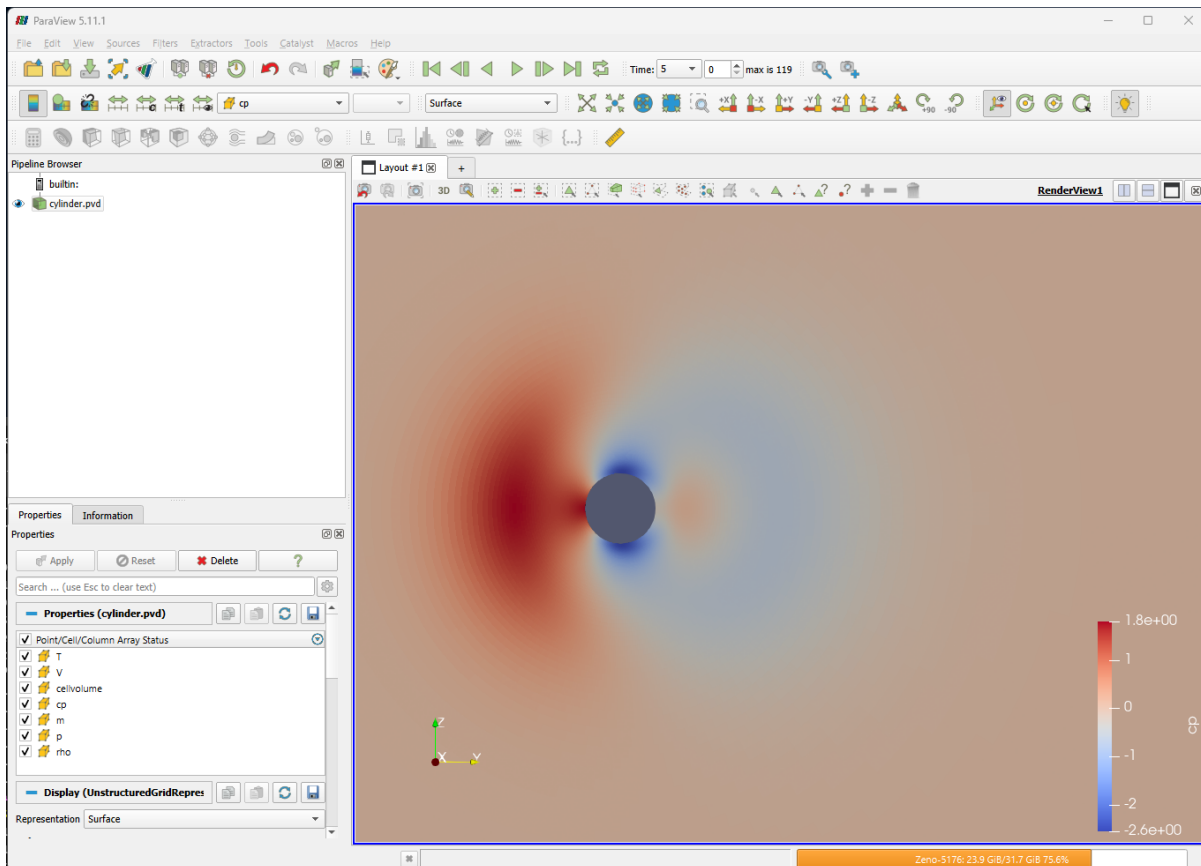
Launch Paraview and load `'cylinder_P1_OUTPUT/cylinder.pvd'`. Paraview will render a single solution time step at a time, and time series data can be navigated using the icons at the top of the screen:



Animation

For unsteady data it is often useful to output an animation of the solution. This can be done in Paraview by either exporting an image per timestep and then using a third party tool to stitch the images into a video or by saving the animation directly. The advantage of the first approach is that it can easily be scripted and is more suitable for large cases. Since this case is quite small we will export an mp4 video directly from Paraview. The steps to do this are:

1. Launch Paraview and load `'cylinder_P1_OUTPUT/cylinder.pvd'`.
2. Set the view up to shade the output by `'cp'` and zoom/move the image until you are happy with the view:



3. Select 'File->Save Animation' in Paraview. To export as video select your preferred format, the format will depend on your Operating System but for Windows you should be able to select "MP4 files" and on Linux "FFMPEG AVI". Give the file a name and click OK.
4. On the next screen you can set the target resolution, frame rate and the timesteps to export. Set the Image resolution to 1920x1080 (FHD) and the frame rate to 24. If you just want to export the end of the simulation (where the oscillation is established) you can set the Frame Window from 300 to 600.
5. Click OK to export the animation. This will take some time.

You should now have an exported video of the unsteady simulation.

1.4.4 Tutorial 5: FWH Solver

A *Ffowcs-Williams Hawkings (FWH) solver*, which is used for prediction of farfield noise, is included in the zCFD distribution. In this section, we will use the zCFD FWH solver to calculate the sound experienced by two 'observer microphones' as a result of the aerodynamic noise generated by the flow around the cylinder.

In order to predict noise at observer microphone locations, an FWH solver requires an initial unsteady CFD solution. We will base our example on the CFD simulation setup from [Tutorial 3](#) with some additional modifications to record the flow variables on an 'FWH surface' in the near-field, noise generating region. We then use the FWH solver to propagate the noise from the near-field FWH surface to the observer microphones.

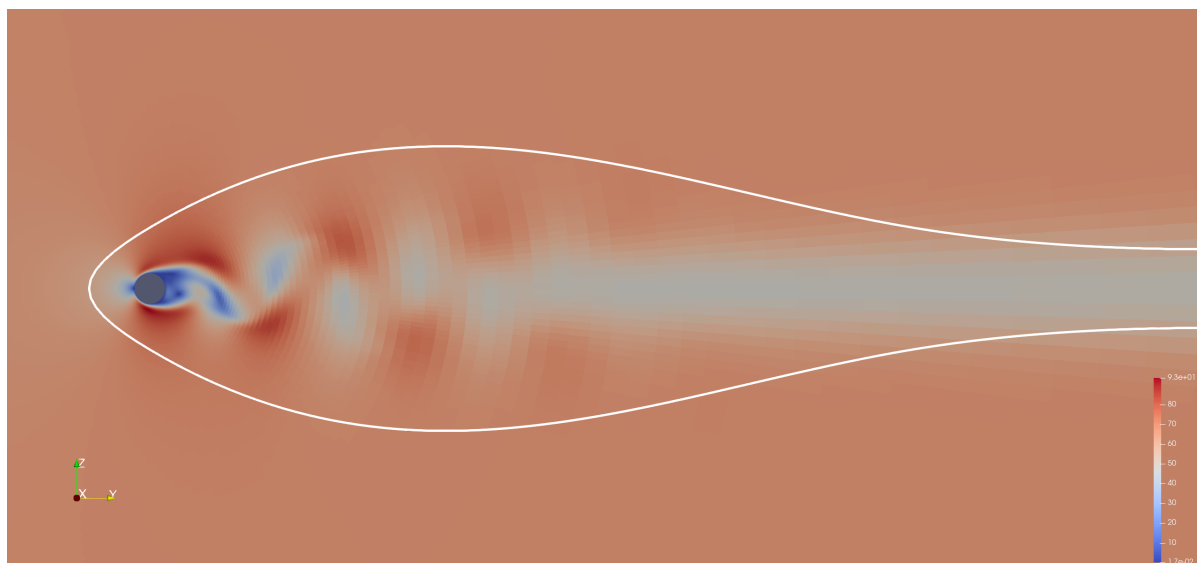
The FWH solver can be run in two ways - the *run_fwh utility* and *fwh python module*. In this tutorial, the simpler *run_fwh utility* is introduced first, followed by the *fwh python module* and postprocessing using a *jupyter notebook*.

Running zCFD with FWH output

The flow we're going to be running the FWH solver on is the shedding cylinder. To get the required inputs to our FWH solver, we need to define an *FWH surface*, and collect data on this surface during a CFD simulation.

The files required for the fwh tutorial can be downloaded [here](#). In the zip file there's a FWH surface definition file, called *fwh_surface1.stl*. Given we've already run the cylinder case in [Tutorial 3](#), we can view the FWH

surface in Paraview alongside the cylinder CFD volume data (see [here](#)), as below. You may find the surface easier to see if you set the *view style* to be *Feature Edges* instead of *Surface* for the FWH surface, and increase the *Line Width* in the *Geometry Representation*.



The FWH surface encloses the noise generating near-field region, but does not intersect the wake, in order to avoid spurious pseudo-sound [1, 2].

There's also a prepared control dictionary, *cylinder_fwh.py*. This is identical to tutorials 3's *cylinder.py* apart from the output section, which is detailed below.

```
"write output": {
  "format": "vtk",
  "surface variables": ["V", "p", "T", "rho", "cp"],
  "volume variables": ["V", "p", "T", "rho", "m", "cp"],
  "fwh interpolate": ["fwh_surface1.stl"],
  "frequency": {
    "fwh interpolate": 1,
    "volume data": 1000,
    "surface data": 1000,
  },
},
```

In this case, we have chosen to output *fwh interpolate* data every single timestep, using the *fwh_surface1.stl* FWH surface definition file. Volume and surface data is much less frequent, since we already have all this data from when we ran *cylinder.py* [above](#).

For the FWH tutorial we have also updated the *'time marching'* section to run the simulation for 4 seconds, rather than 1.2. We run the CFD simulation in the normal way, using the command below.

```
run_zcfd -m cylinder.h5 -c cylinder_fwh.py
```

When we've run the CFD simulation of the cylinder, we should be able to see the FWH interpolated data in *'cylinder_fwh_P1_OUTPUT/ACOUSTIC_DATA/fwh_surface1_FWHData.h5'*. There is also a corresponding *xdmf* file, *'cylinder_fwh_P1_OUTPUT/ACOUSTIC_DATA/fwh_surface1_FWHData.xdmf'*, which allows us to open the FWH surface in Paraview and see the pressure, velocity and density at each cell centre varying with simulation time. Use the Paraview *Time* controls to adjust the simulation time being viewed. You may find that changing the *view style* to *Point Gaussian* and increasing the *Gaussian Radius* in the *Properties* sidebar makes the cell values easier to see.

Running the zCFD FWH solver

Using the `run_fwh` utility

We're going to use the `run_fwh` utility to calculate noise at an observer `Obs1`. '`Obs1`' is an observer that is a fixed distance away from the cylinder - if we consider the cylinder in a wind tunnel, we could consider '`Obs1`' as a microphone attached to the wind tunnel wall. Since `Obs1` is static relative to the FWH surface, it is in the same *translational reference frame* as the FWH surface and we can therefore use the `run_fwh` utility.

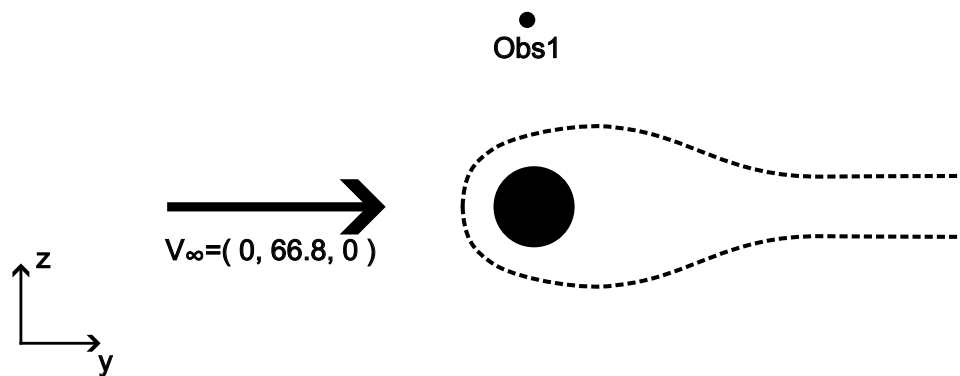


Fig. 1.1: FWH surface and `Obs1` motions - CFD frame of reference

To use the `run_fwh` utility we need three inputs - a *zCFD control file*, a *reference condition* specification and an *observers.csv file*.

The zCFD control file is simply the control file for the zCFD simulation we used to create the FWH surface data - in this case, `cylinder_fwh.py`. `run_fwh` reads `cylinder_fwh.py` and can see that we have a single FWH surface, with data stored at '`cylinder_fwh_P1_OUTPUT/ACOUSTIC_DATA/fwh_surface1_FWHData.h5`'.

Next, we have to define a *reference condition*. In external flow simulations of this type, the *run_fwh reference condition* is the freestream conditions, defined as a zCFD *IC block*. In this case, the freestream conditions are already defined in `cylinder_fwh.py` to define the farfield boundary condition, so we can simply use '`IC_1`' for the `run_fwh` reference condition.

Lastly, we need to define the name and location of our observers in a `.csv` file. The centre of the cylinder in the CFD mesh is at (0.25,0,0), and we want `Obs1` to always be (0,0,20) metres away from the cylinder centre during the FWH simulation. The file `Observers.csv` (included in the tutorial *.zip file*) therefore contains the following:

```
Obs1, 0.25, 0.0, 20.0
```

Having decided on our inputs, we run the `run_fwh` utility by simply typing the following command within the *zCFD command-line environment*.

```
run_fwh -c cylinder_fwh.py --reference_condition IC_1 --observer_locations Observers.
-csv
```

Running this command prints output to screen and to the `cylinder_fwh.fwh.log` file, and outputs the FWH calculated pressure history at `Obs1` to `cylinder_fwh.fwh.Obs1.csv`. In the case where there are multiple noise sources, the contribution of noise to each source is broken out, with the total observed noise also reported. Suggested post-processing is introduced *below*.

Using the fwh python module

As can be seen above, the `run_fwh` utility is very easy to use and is applicable in most simple FWH calculations. However, it has limitations - namely the fact that all observers and surfaces must be in the same *translational reference frame*, and that using it when more than one FWH surface encloses a noise generating region will *lead to double accounting*.

Where the `run_fwh` utility is not applicable, the *fwh python module* can be used instead. In this section, we will use the *fwh python module* to calculate observer pressure histories at both *Obs1* and *Obs2*, where *Obs2* is a ‘flyby’ observer whose pressure history cannot be calculated using the `run_fwh` utility.

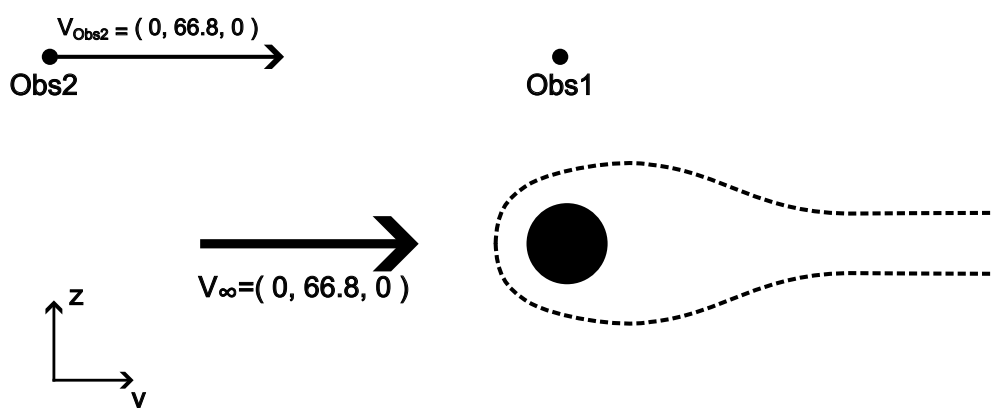


Fig. 1.2: FWH surface and observer motions - CFD frame of reference

FWH Observer and surface motions

When the FWH equations are derived, we make an important assumption - that of a ‘quiescent medium’ (i.e. still air, with a free-stream velocity of zero). Clearly, with a freestream velocity of $(0, 66.8, 0)$, the flow in our CFD simulation does not satisfy this condition. In order to use the FWH solver, we therefore have to perform a co-ordinate transformation, as in Fig. 1.3. In the `run_fwh` utility, this co-ordinate transformation is performed automatically, whereas in the *fwh python module* we set up the surface and observer motions through the FWH quiescent medium manually.

In this ‘quiescent medium’ co-ordinate system, the cylinder and ‘*Obs1*’ are ‘flying’ through the air. In this co-ordinate system, we can also see that ‘*Obs2*’ represents a microphone fixed to the ground, as the cylinder flies overhead.

Setting up the FWH solver inputs

Now that we know the motions of our observers and surface, we can run the FWH solver. The python code required to run the FWH solver is in the file ‘`run_fwh_solver.py`’, and also written out below. We define the surfaces, observers and the solver settings, then use `fwh.solve()` to actually run the FWH solver.

```
from fwh import fwh, motion
import json
import math

# FWH surface motion
```

(continues on next page)

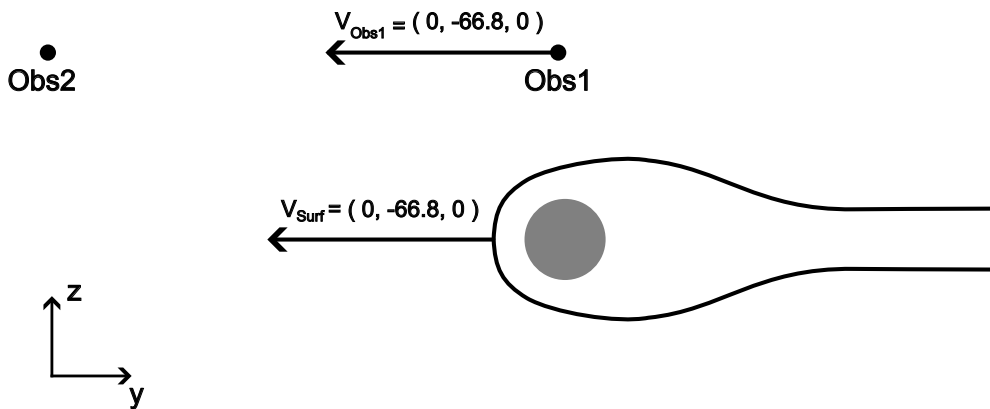


Fig. 1.3: FWH surface and observer motions - FWH (quiescent medium) frame of reference

(continued from previous page)

```

c = math.sqrt(1.4 * 277.7777 * 287)
v_surf = [0, - 0.2 * c, 0] # = [0, -66.8, 0]
surfaceCentrePoint = motion.ConstantVelocityPoint([0.0, 0.0, 0.0], v_surf)
surfaceMotion = motion.NonrotatingSurface(surfaceCentrePoint)

# obs1 motion - [0,0,20] above cylinder centre
obs1_CFD_frame_posn = [0.25,0,20]
obs1Motion = motion.ConstantVelocityPoint(obs1_CFD_frame_posn, v_surf)

# obs2 motion - stationary, intersects with obs1 at t=2.5
obs2_posn = []
for i in range(3):
    obs2_posn.append( obs1_CFD_frame_posn[i] + 2.5* v_surf[i])
obs2Motion = motion.StationaryPoint(obs2_posn)

solverSettings = {
    "c": c,
    "dt": 0.002,
    "rho0": 101325.0 / (277.7777 * 287),
    "p0": 101325.0,
}

surfaces = {
    "surf1": {
        "motion": surfaceMotion,
        "fileName": "./cylinder_fwh_P1_OUTPUT/ACOUSTIC_DATA/fwh_surface1_FWHData.h5",
    }
}

observers = {"Obs1": obs1Motion, "Obs2": obs2Motion}

pOut, tOut = fwh.solve(surfaces, observers, solverSettings)

```

(continues on next page)

```
dataForJson = {"p": pOut, "t": tOut}

with open("./FWH_data.json", "w") as f:
    json.dump(dataForJson, f)
```

More details on FWH solver setup can be found [here](#), but the most important concept is that we use ‘*motion classes*’ to define observer and surface motions. The available *point (observer) motions* are ‘*OriginPoint*’, ‘*StationaryPoint*’ and ‘*ConstantVelocityPoint*’. The available *surface motions* (which rely on a *point motion* to define the motion of their centre) are ‘*NonrotatingSurface*’ and ‘*RotatingSurface*’.

The velocities and fluid properties used in the FWH simulation are taken from the ‘*cylinder.py*’ zCFD control file. `solverSettings['dt']` has been set to be the same as the timestep between outputs in the FWH surface data (0.002 seconds, see [above](#)).

In general, we can consider the motion of a point on an FWH surface to be defined by $\mathbf{x}(t) = \mathbf{x}_0 + \mathbf{V}_{surf} t$ in the FWH co-ordinate frame. \mathbf{V}_{surf} is defined by the user in the *surface motion class* (called *surfaceMotion* above) and \mathbf{x}_0 is the position defined by the FWH surface definition file (‘*fwh_surface1.stl*’, see [above](#)).

The centre of the cylinder in the CFD mesh is at (0.25,0,0), and we want *Obs1* to always be (0,0,20) metres away from the cylinder centre during the FWH simulation. Since the cylinder ‘travels with’ the FWH surface (see [Fig. 1.3](#)), we can therefore say that the motion of the cylinder centre in the FWH co-ordinate frame is $\mathbf{x}(t) = (0.25, 0, 0) + (0, 0, 20) + \mathbf{V}_{surf} t$. We therefore set the motion of *Obs1* to be $\mathbf{x}(t) = (0.25, 0, 20) + \mathbf{V}_{surf} t$. We set *Obs2* to be stationary in the FWH reference frame, and to be coincident with *Obs1* at $t=2.5$. We save the outputs to a json file called *FWH_data.json*.

Running the FWH solver

The python code above is replicated in ‘*run_fwh_solver.py*’. To run the FWH solver, we simply run the command below from within the *zCFD command-line environment*. You may need to change the `surfaces["surf1"]["fileName"]` parameter depending on how many ranks you used in your zCFD run.

```
python3 run_fwh_solver.py
```

This will output various information to the screen, including the ‘valid min and max times’ for each surface / observer combination.

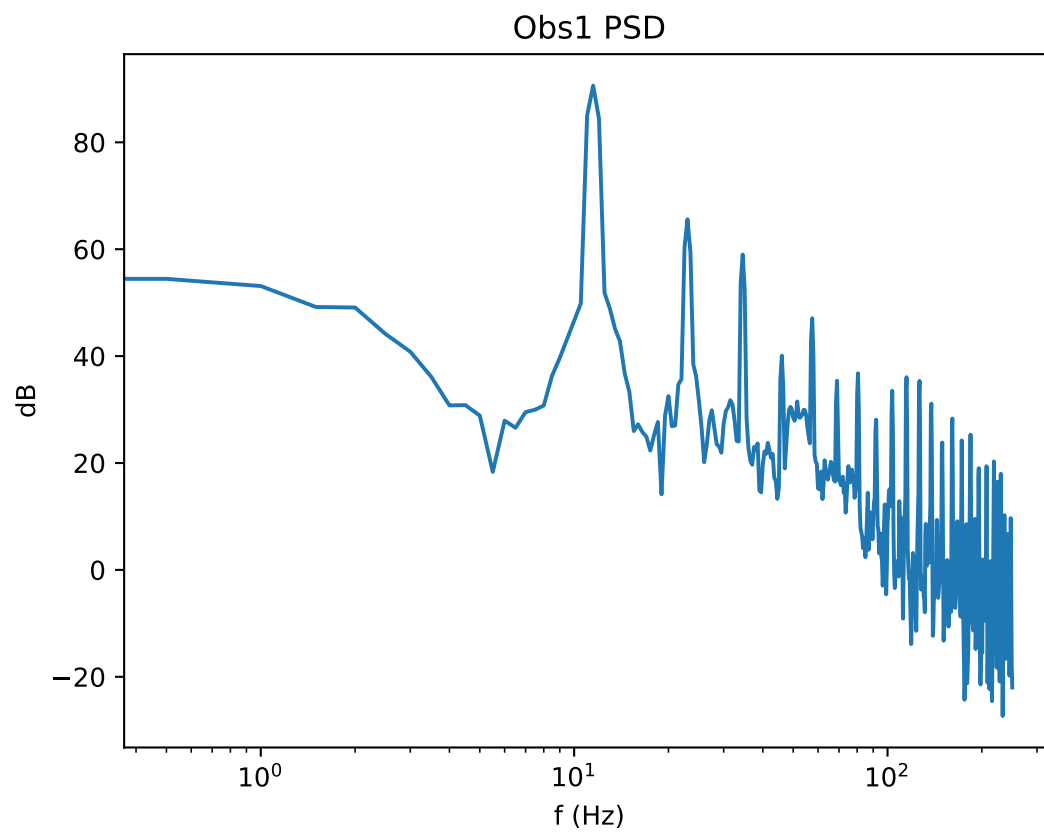
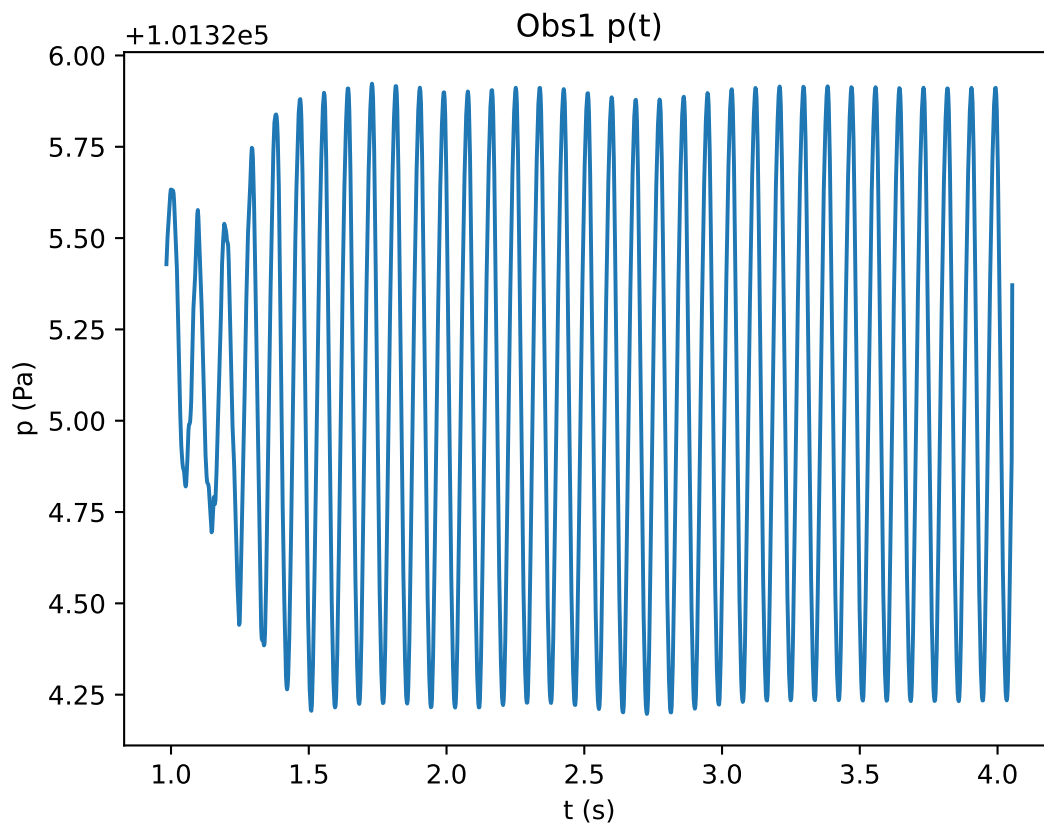
The valid min and max times denote the time window during which an observer receives data from all points on the FWH surface. A pressure signal emitted from a point on the FWH surface at time t takes r/c seconds to arrive at an observer, where r is the distance from the surface point to observer and c is the speed of sound. Therefore the valid observer time window will always be later than the FWH surface output time window (in our case, 0.002:1.2 seconds) due to the distance from the FWH surface to the observer. The valid observer time window will be narrower if the FWH surface is large, since the larger the surface the larger the time delay between signals from different points on the surface reaching the observer becomes.

Post-processing

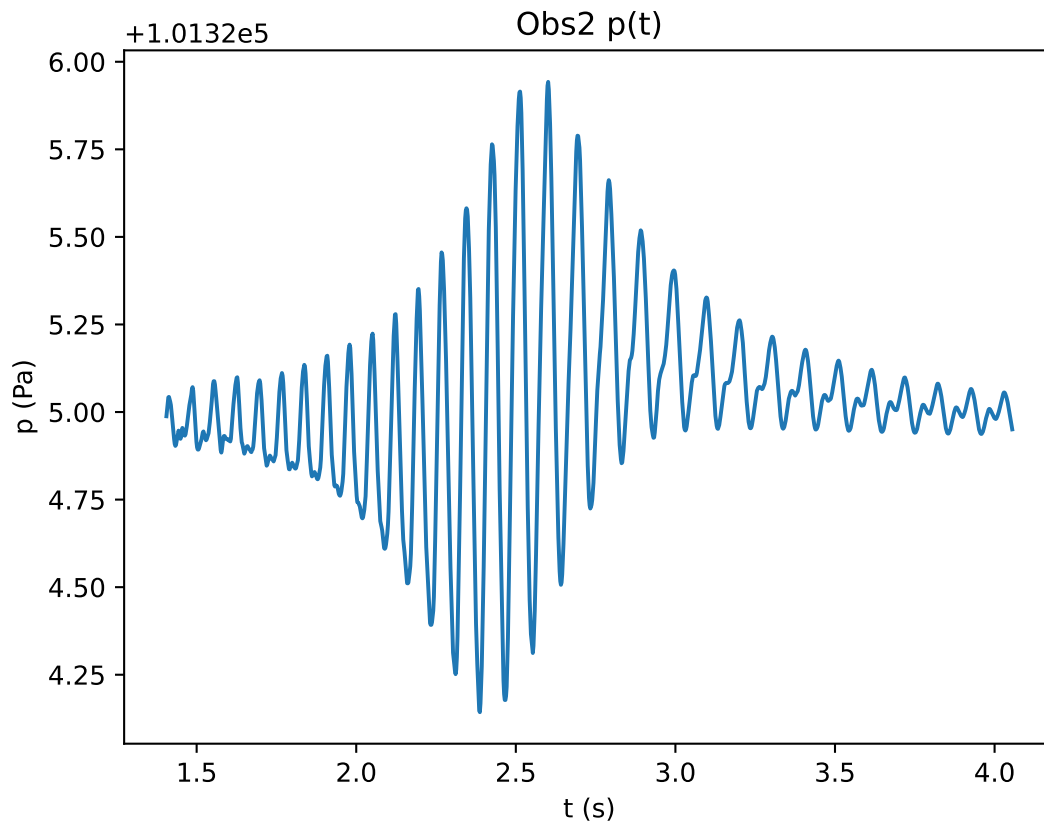
The *jupyter notebook* *postprocess_fwh_module_data.ipynb* from the *.zip file* can be used to post-process the FWH data. *postprocess_fwh_module_data.ipynb* uses the data from the *fwh python module section* of this tutorial, but an equivalent notebook which uses the data from the *run_fwh utility section* is available in *postprocess_run_fwh_data.ipynb*.

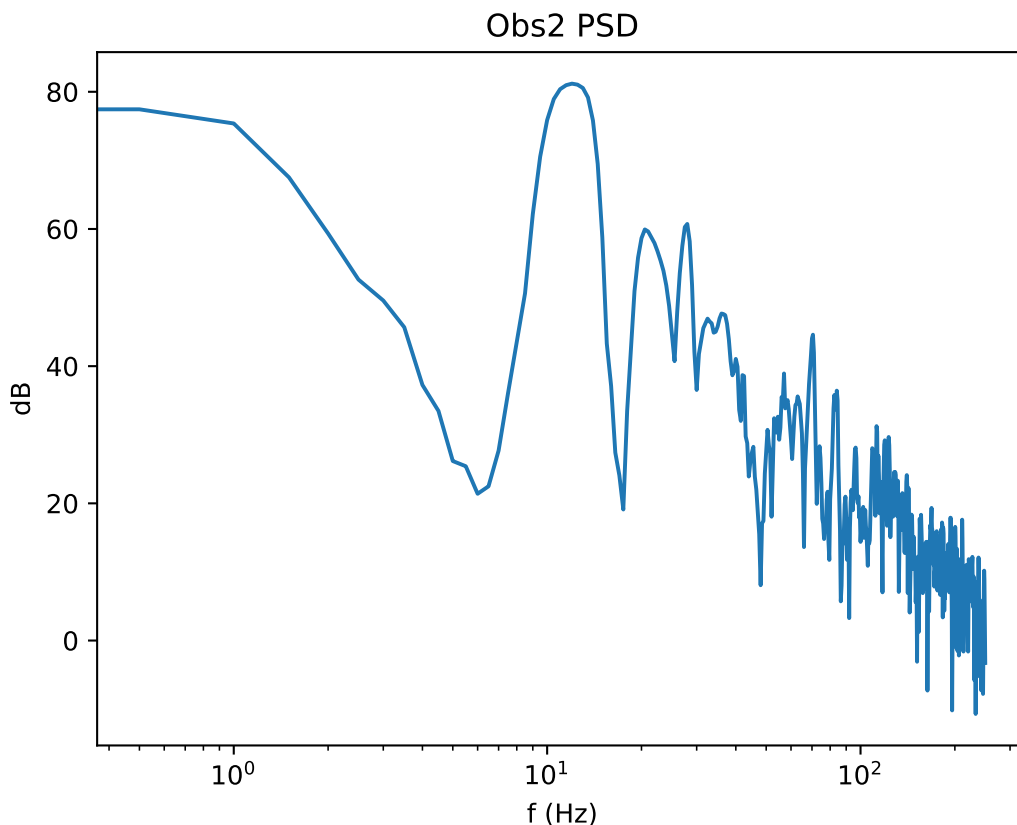
These notebooks contain a number of *zutil* functions which may be useful for users wishing to perform acoustic post-processing. The notebooks plot the pressure history $p(t)$ and power spectral density (PSD) at both observers, as below.

Obs1 moves through the FWH medium at a constant displacement from the cylinder centre (see [Fig. 1.3](#)). We see from our post-processing that the noise experienced by *Obs1* is dominated by a constant 10 Hz component, which is the shedding frequency of the cylinder. Various harmonics of the 10 Hz signal are present in the power spectral density plot for *Obs1*.



During the FWH simulation run in the *fvh python module section* of this tutorial, the cylinder gets closer to *Obs2* from 0 to 2.5 seconds, before getting further away from *Obs2* from 2.5 seconds onwards. We can see in the *Obs2 p(t)* plot that the peaks are closer together from 0 to 2.5 seconds than they are after 2.5 seconds. This is due to Doppler shift. We can also see the effect of Doppler shift in the power spectral density, which has a more rounded 10 Hz peak than that seen in *Obs1*.





`postprocess_fwh_module_data.ipynb` also creates `.wav` files, which allow you to listen to the sound experienced by `Obs1` and `Obs2`.

Extensions

To become more comfortable with the FWH solver, various extensions to this exercise are possible. Here are some suggestions.

1. Re-run the zCFD solver, but this time extract FWH data on the cylinder *wall* instead of `fwh_surface1.stl`. Run the FWH solver (using the wall data as an *impermeable* FWH surface) and compare the results to those achieved using the `fwh_surface1` permeable FWH surface.
2. Re-run the zCFD solver, but this time also extract FWH data on the `fwh_surface2.stl` and `fwh_surface3.stl` surfaces. These are like `fwh_surface1.stl` but slightly larger. Run the FWH solver with these surfaces and investigate the effect of using different surfaces on the FWH results. You will have to do this using the `fwh` python module to avoid *double accounting*.
3. Add extra observers of your choice to the FWH solver.
4. Use the file utility `writeFWHSurfaceFrequenciesFile` to visually inspect the spatial distribution of different frequencies in the FWH surface.
5. Use the file utility `writeBlankedOffFwhSurfaceFile` to ‘blank off’ all FWH surface cells more than 5 cylinder diameters downstream of the cylinder’s centre. Run the FWH solver using this modified surface, and based on this estimate how much of the shedding noise originates more than 5 diameters downstream of the cylinder.
6. Use the `solver.fwh_helper_functions` module to rewrite `run_fwh_solver.py` so that the `solverSettings` dictionary is automatically set based on the zCFD control file name and reference condition which were used in the `run_fwh` utility.

Note

Since the cylinder CFD simulation is '2.5D' (i.e. the mesh only has a single cell in the x direction), the distance scaling of $p(t)$ at observers will be non-physical.

Citations

1. Mitchell, B., Lele, S., & Moin, P. (1999). Direct computation of the sound generated by vortex pairing in an axisymmetric jet. *Journal of Fluid Mechanics*, 383, 113-142. [10.1017/S0022112099003869](https://doi.org/10.1017/S0022112099003869)
2. Ricciardi, T. R. , Wolf W. R. , & Spalart P. R. (2022). On the Application of Incomplete Ffowcs Williams and Hawkings Surfaces for Aeroacoustic Predictions. *AIAA Journal*, 60:3, 1971-1977. [10.2514/1.J061285](https://doi.org/10.2514/1.J061285)

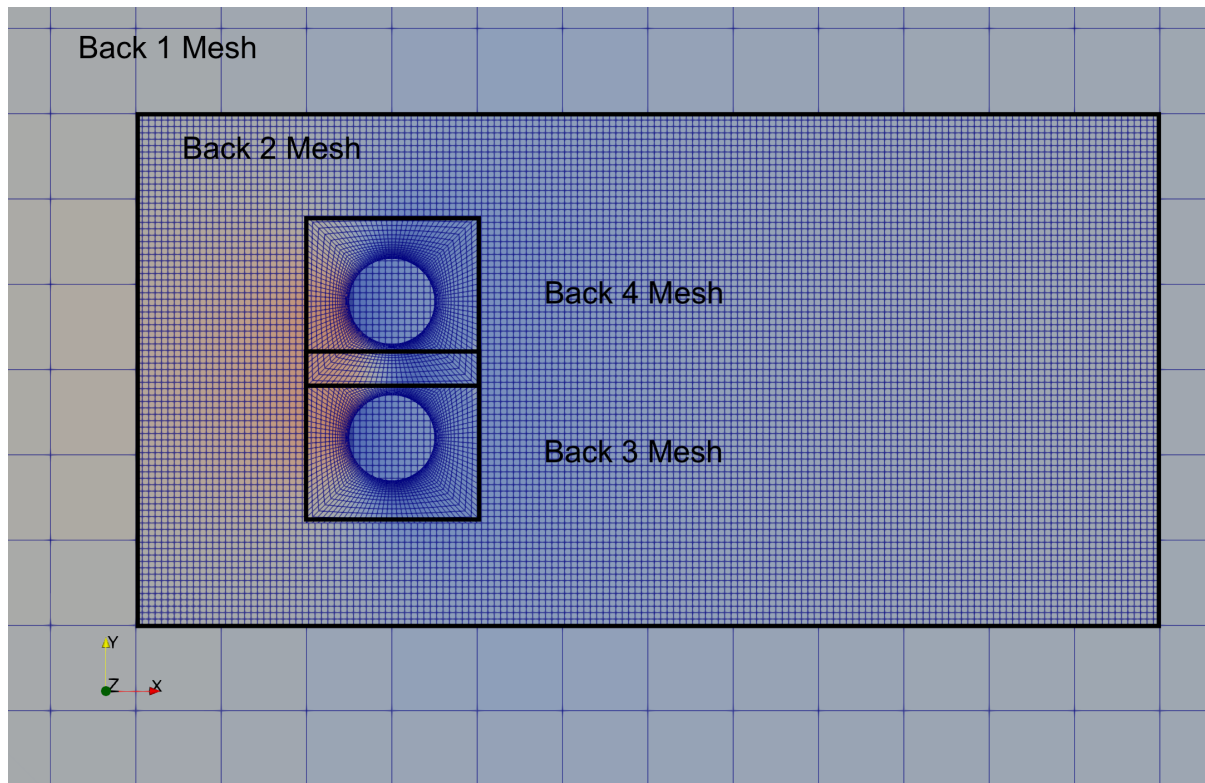
1.4.5 Tutorial 6: Overset Meshes

There are various situations in CFD modelling when it is useful to be able to place one mesh over the top of another one, effectively blanking out the cells in the lower level mesh in favour of the mesh on top, while maintaining solution accuracy across the interface.

- We may want a higher order of solution accuracy in a region of the original finite volume mesh. The overset mesh would be designed for a higher order simulation than elsewhere in the flow domain.
- We may want to include a component in a simulation that is not part of the original mesh. For example, we may want to add a rotating component to a static mesh. The overset mesh would be designed for the rotating component, and would be placed over the static mesh.
- A specific mesh may already exist for a rotating component (such as a propeller) that we want to be able to easily add to models of different aircraft without having to re-create the propeller mesh. The propeller meshes (there may be several) are overset on the aircraft mesh, allowing for a fully coupled solution.
- There may be components in relative motion, such as a train entering a tunnel. In this case the mesh for the train can overset the background mesh for the tunnel, and the train can move into the tunnel without the need for any new mesh generation. The solver takes care of the changing mesh mapping across the boundary as the train moves, including preservation of the solution accuracy with a region of overlapping meshes.
- There may already be a high quality mesh for an aircraft or a cityscape, and we want to include a new component or a new building without regenerating the entire mesh. It may be simpler to include any changes into a new mesh of a small region, and apply it like a patch as an overset mesh.

This is called an overset mesh technique, and is supported by zCFD. In all cases, the flow solutions are calculated separately on each mesh, with the solver managing the interfaces and interpolation accuracy. zCFD will support different solution methods, different orders of spatial accuracy on each mesh, and arbitrarily large numbers of overset meshes in each simulation. The order of the sequence of meshes specified by the user determines which mesh is active in each part of the flow domain. zCFD automatically manages the data exchange between all meshes, including parallel partitions.

Example 1 - Multiple Overset Cylinder Test Case



There are 4 (mesh, control dictionary) pairs of input files. These are listed in a special “override” file called “oversetmulticylinder.py” used for overset cases:

```
override = {'mesh_case_pair': [ ('back1.h5', 'back1'),
                                ('back2.h5', 'back2'),
                                ('back3.h5', 'back3'),
                                ('back3.h5', 'back4') ]}
```

Note that in this case, the “back3.h5” mesh defining a cylinder has been used twice. This is OK, because the “back3.py” and “back4.py” control dictionaries each apply a different transformation (down and up along the y-axis respectively). The solver knows that the meshes are used for different solutions, in different parts of the flow domain. Also note that the translated mesh for “back4” overlaps the translated mesh for “back3” (the mesh between the two cylinders). This is also OK because the solver knows that “back4” oversets “back3”, which oversets “back2” and “back1”. In each case, the active solution is the one on the top-level oversetting mesh.

The files for running the case are available for download [here](#).

For each of the meshes, a transformation has been defined in the corresponding control file, for example the “back1.h5” mesh is moved according to the transformation defined by the following lines in the “back1.py” control dictionary:

```
"mesh transform matrix": zutil.transform.translate(
    [0.0, 0.0, 0.0], [0.0, 0.0, -1.5]
),
```

This tells the solver to use the inbuilt transformation function in zutil to translate the mesh down in the z-axis by 1.5 units. The lowest level mesh (i.e. that does not overset any other meshes) does not require any other modification, providing that the order of solution spatial accuracy supported by the meshes that overset it are that same as its own accuracy. For all of the meshes that overset at least one other mesh, a special boundary condition must be applied to any zone (boundary) where information is to be exchanged between meshes. For example, in “back3.py” the following line is used:

```
"BC_2": {"zone": [13], "type": "overset"},
```

For the “back3.h5” mesh, zone 13 (comprising boundary faces excluding symmetry planes and the cylinder surface) is designated as an overset boundary. This means the solver will interpolate and exchange data between this zone and the background mesh (“back2.h5”). The software automatically calculates the necessary mapping and interpolation coefficients to preserve the spatial accuracy of the overset solution.

The “Multiple Overset Cylinder” test case runs in a few minutes on a GPU, with the simple command:

```
run_zcfd -f oversetmulticylinder.py
```

The usual command line arguments specifying the mesh and the case name are not required as they are replaced with the list in the “override” dictionary specified within the “oversetmulticylinder.py” file.

When complete, the following outputs should be produced:

```
back[1,2,3,4]_P1_OUTPUT  
back[1,2,3,4]_report.csv  
back[1,2,3,4]_results.h5  
back[1,2,3,4]_status.txt  
oversetmulticylinder.log  
oversetmulticylinder_report.ipynb
```

Where the [1,2,3,4] indicates that the file or directory exists for each overset solution separately. From a post-processing perspective, overset grids offer a significant advantage: independent solutions that only exchange boundary data during computation. This independence can save post-processing time and memory, as not all solution files are needed to analyse specific regions. However, a separate step is necessary to combine these independent solutions for domain-wide processing, such as extracting cross-sections. ParaView can be used to illustrate this combination process.

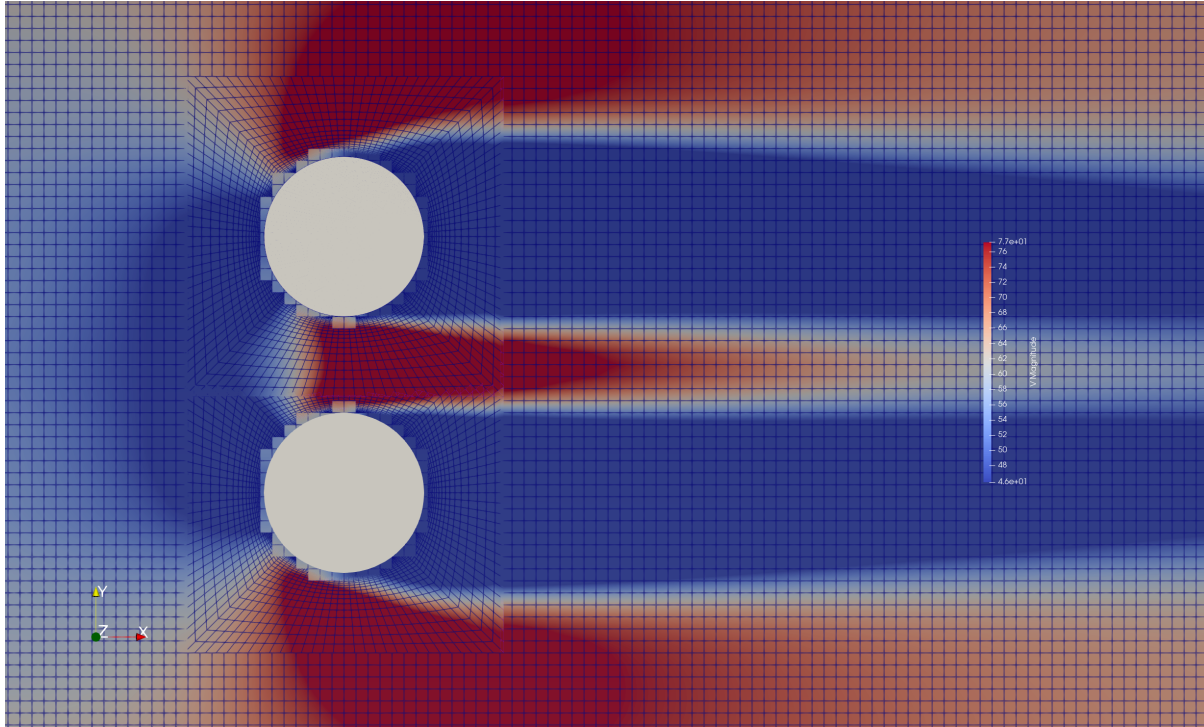
Post-processing using ParaView

To combine the 4 overset meshes into a single solution that can be operated on as though it were a single object, we use the “Append Datasets” filter in ParaView.

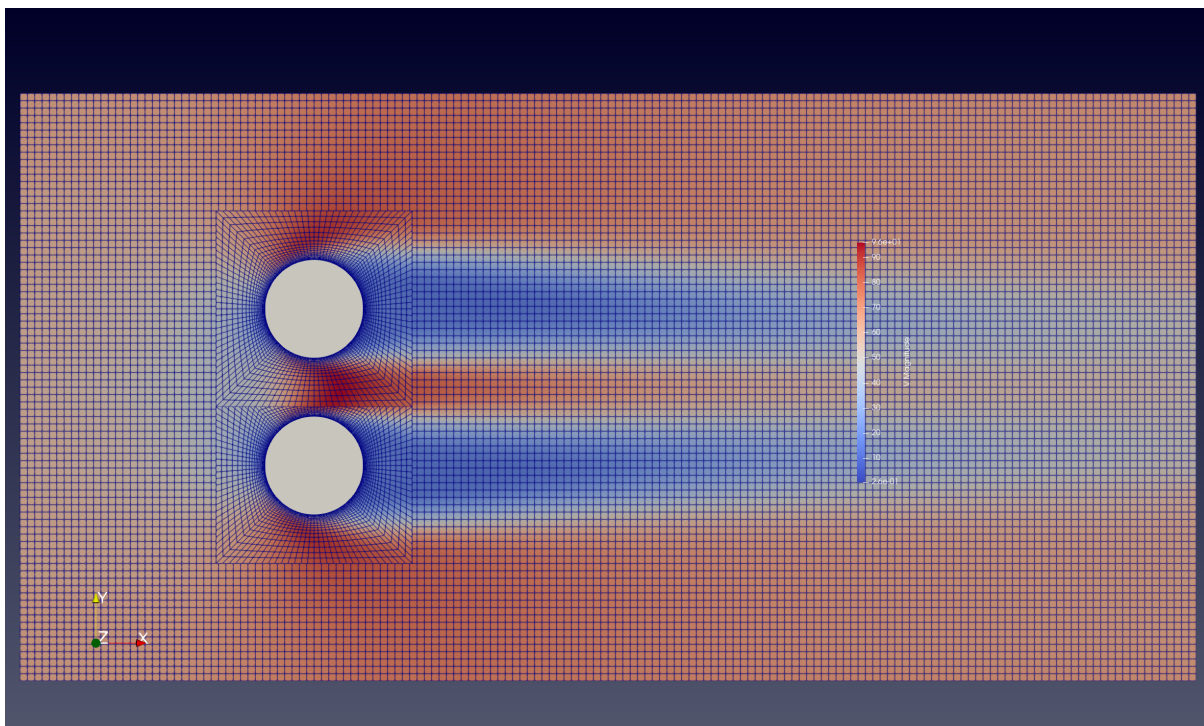
- Launch ParaView so that you can load the solution files (locally or remotely).
- Load the 4 files “back*_P1_OUTPUT/back*.pvd” for * = 1,2,3 and 4.
- Highlight all 4 files on the navigation tree (on the left) and select “Filters > Append Datasets”. This will create a new item in the navigation tree called “AppendDatasets1” that acts on all four datasets at once.
- The volumetric data output for this case contains a variable called “overset” which is 0 or 1 for any cell in the meshes. 0 means that the cell has been overset by another mesh, and 1 means that the cell is the active cell in that location. Use the “Filters > Threshold” filter to select only the cells in the “Append-Datasets1” combined dataset that have an “overset” value of 1 (do this by changing the lower threshold value from 0 to 1). This will create a new item in the navigation tree called “Threshold1” excluding any cells that have been overset by cells in another mesh.
- Use the “Filters > Cell Data to Point Data” filter to interpolate the cell data from “Threshold1” to the mesh nodes. This makes subsequent interpolation operations in ParaView more accurate. This will create a new item in the navigation tree called “CellDatatoPointData1”.
- Use the “Filters > Slice” filter to extract the solution from “CellDatatoPointData1” onto a plane with normal in the “Z” direction. Note that this contains data from all 4 meshes.
- Colour the new “Slice1” object by “V” “Magnitude”, selecting “Surface With Edges” in the visualisation toolbar.

Other post-processing steps such as streamlines or animations will also work with overset meshes in the same manner. If the meshes are in relative motion throughout an unsteady simulation, ParaView will automatically update their positions.

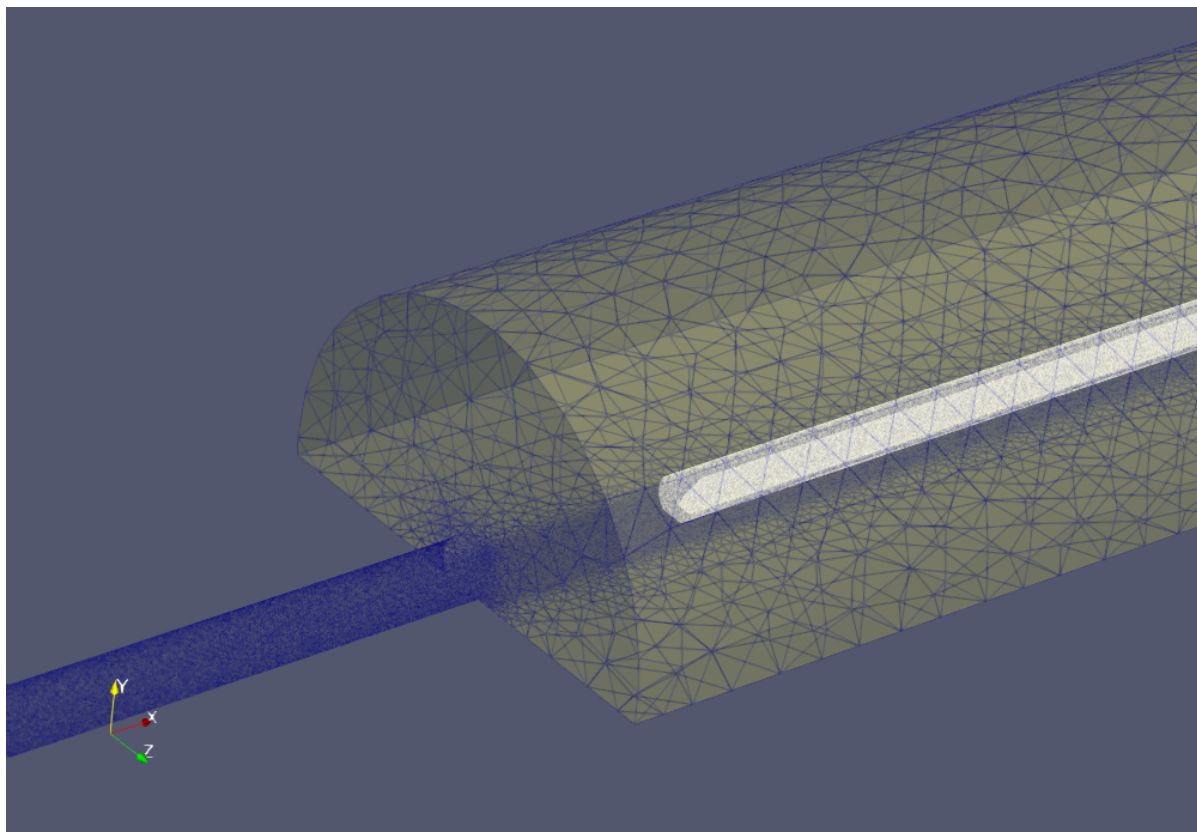
- [Optional] The “back2” solution will show through behind the “back3” and “back4” overset solutions because of the holes where the cylinders are. Any solution is non-physical, and an easy way to mask this effect is to insert some simple geometry to show the location of the cylinders. Use “Sources > Cylinder” to create a unit diameter cylinder at $[0,0,0]$ and rotate it 90 degrees about the x-axis, then translate it in the y-axis by -0.8 in y to put it into place. Repeat, but with a translation of $+0.8$ for the other cylinder.
- [Optional] The above steps will produce the image below:



To create the image in the validation page, you can force ParaView to bring the overset meshes to the foreground by treating each of the overset meshes independently, and adding a small incremental offset normal to the slice plane to each cylinder mesh (0.0, 0.001, 0.0015, 0.002). This will better reflect what the solver will actually see, as the overset cells in the background meshes will not be active.



Example 2 - Train Tunnel Test Case



This test case demonstrates the zCFD overset capabilities to predict the micro pressure wave generated as a train enters a tunnel, and is a good example of a practical application of overset meshing. The simulation set up follows that described in Section 7.6 of Railway applications — Aerodynamics — Part 5: Requirements and test procedures for aerodynamics in tunnels. In order to avoid transients, the train is linearly accelerated from 0 to 250 km/hr over 1.5 seconds.

For the reference train entering the reference tunnel at 250 km/hr, the maximum entry pressure gradient dp/dt should be in the range of 8800 Pa/s to 9500 Pa/s. These values are used to validate the simulation.

The input control dictionary for the train in this case also shows how to programmatically define the motion of a mesh in time:

```
def linear_accel(**kwargs):
    t = kwargs["time"]
    dt = kwargs["time step"]
    u = [-69.4, 0, 0]
    if t < 1.5:
        u[0] = -(t / 1.5) * 69.4
    return {"velocity": tuple(u)}
```

This function returns the velocity to be applied to a fluid zone, which is then defined by:

```
'FZ_1' : {
    'type' : 'translating',
    'zone' : [6],
    'vector' : [-1,0,0],
    'mach': 69.4 / math.sqrt(1.4 * 287 * (277.7777 + 15)),
    'translation function': linear_accel,
},
```

The motion is applied to the mesh because of the keyword 'moving mesh' in the 'time marching' section of the

control dictionary. This will force a recalculation of the physical location of the mesh, including the recalculation of any overset mappings, every real time step.

```
"time marching": {
    "unsteady": {"total time": 3.6,
                 "time step": 0.001,
                 "order": 1, "start": 0},
    "scheme": {"name": "implicit euler", "stage": 1},
    "cfl": 30,
    "cycles": 5,
    "moving mesh": True,
},
```

The meshes and control files for the train and the tunnel can be downloaded from [here](#).

The train tunnel case is larger than the previous case in this tutorial: the train mesh has 1.31m cells and the tunnel has 7.35m cells. To run this case in implicit mode on a GPU will require approximately 48GB RAM.

The case can be run with the command

```
run_zcfd -f override_roe.py
```

Post-processing

To plot the entry pressure gradient over time, copy the following Python code into a file 'create_plot.py':

```
# Compute maximum entry pressure gradient dp/dt
import matplotlib.pyplot as plt

ts = 0.001
file_name = "tunnel_roe_report.csv"
p_data = []
with open(file_name) as fp:
    line = fp.readline().split()
    count = 0
    val = 0
    while line:
        line = fp.readline().split()
        if len(line) > 0:
            c = int(line[0])
            if c != count:
                count = count + 1
                val = float(line[7])
                p_data.append(val)

    p_grad_data = []
    time = []
    for i in range(len(p_data)-1):
        if ts*i < 4:
            p_grad_data.append((p_data[i+1] - p_data[i]) / ts)
            time.append(ts * i)

plt.minorticks_on()
plt.grid(which="both")
plt.title('Maximum entry pressure gradient = '+str(round(max(p_grad_data),6))+' Pa/s')
plt.xlabel("Time [s]")
plt.ylabel("dPdt [Pa/s]")
plt.xlim(0, 3.6)
plt.ylim(-100, 12000)
```

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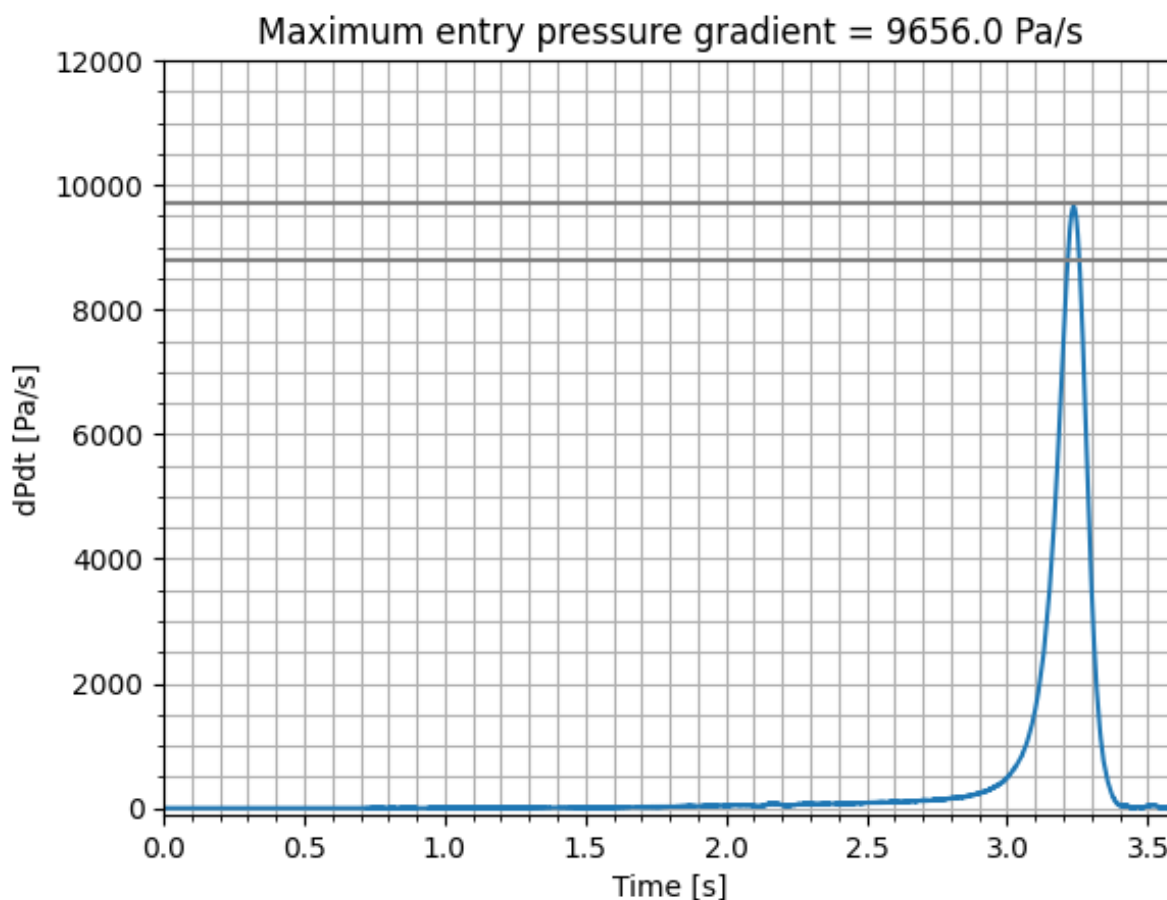
(continued from previous page)

```
plt.plot(time, p_grad_data, label="250km/hr @ 15oC")
plt.plot([time[0],time[-1]], [8800,8800], label='min valid dP/dT', c='grey')
plt.plot([time[0],time[-1]], [9700,9700], label='max valid dP/dT', c='grey')
plt.show()
plt.savefig("EntryPressureGradient.png")
plt.close()
```

Then run the code in the same directory as the solution files with the command:

```
python create_plot.py
```

This will create the following plot, showing the maximum entry pressure gradient as a function of time. The maximum entry pressure gradient is 9656.0 Pa/s, which is within the range of values specified [8800.0, 9700.0] in the standard.



Citations

1. EN 14067-5:2006 - Railway applications - Aerodynamics - Part 5: Requirements and test procedures for aerodynamics in tunnels, See <<https://standards.iteh.ai/catalog/standards/cen/ea6cb49e-c40a-4b8b-a059-c6debbdb91dc7/en-14067-5-2006>>

1.5 Reference Guide

The zCFD control file is a python file that is executed at runtime. This provides a flexible way of specifying key parameters, enabling user defined functions and leveraging the rich array of python libraries available.

A python dictionary called 'parameters' provides the main interface to controlling zCFD

```
parameters = {...}
```

zCFD will validate the parameters dictionary specified at run time against a set of expected values for each key. In general, values that should be integers and floats will be coerced to the correct type. Values which should be strings, booleans, lists or dictionaries will cause an error if they are the incorrect type. The time marching scheme and solver/equation set chosen defines which dictionary keys are valid. A simple script is provided to allow the user to check the validity of their input parameters before submitting their job. See [Input Validation](#).

This reference guide documents the parameters available in a zCFD control dictionary and the valid values for those keywords.

```
parameters = {
  'reference': IC_1,
  'initial': {Initial State},
  'restart': False,
  'partitioner': 'metis',
  'scale': [1,1,1],
  'time marching': {Time Marching},
  'linear solver settings': {Linear Solver Settings},
  'equations': {Equations},
  'material': {Material Specification},
  'IC_1': {Initial Conditions}
  'BC_1': {Boundary Conditions}
  'FZ_1': {Fluid Zones}
  'TR_1': {Mesh Transformation}
  'mapping': {Overset}
  'write output': {Write Output}
  'report': {Reporting}
}
```

1.5.1 Reference Settings

Reference state

Keyword	Re-quired	Default	Valid values
'reference'	No	'IC_1'	"IC_?" where ? is an integer.

```
# set reference state to IC_1
'reference': 'IC_1',
```

Sets the *Initial Condition* which provides the reference quantities when non-dimensionalisation is applied to *force reporting*. "IC_?" must be a valid *initial conditions* dictionary defined in the parameters file

Initial State

Keyword	Re-quired	Default	Valid values
'name'	No	'IC_1'	"IC_?" where ? is an integer.
'func'	No	-	An (optional) <i>initial conditions function</i> .

```
# set initial state to IC_1
"initial": {
```

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```
"name": "IC_1"
}
```

Sets which block *Initial Condition* block will be used to provide initial flow field conditions for the simulation. If 'func' is provided it will be used to provide the initial flow field variables on a cell-by-cell basis.

Note

If the 'initial' entry is missing then the conditions default to the *reference* state.

Scale mesh

Keyword	Re-quired	Default	Valid values
'scale'	No	[1,1,1]	[scaleX,scaleY,scaleZ] : Any list of positive floats with length 3

Before being loaded in to the solver, the mesh's [x,y,z] location data is multiplied by this vector.

Example usage:

```
# Scale from mm to metres
'scale': [0.001,0.001,0.001]
```

```
# Scale from inches to metres
'scale': [0.0254,0.0254,0.0254]
```

```
# Scale the mesh to be 10 times larger in y axis
'scale' : [1,10,1]
```

Note

The 'scale' parameter applies to the mesh only - not interpolated surface outputs etc. (see *Tab x*). When a mesh transform matrix is supplied as well as a scaling the scale is applied after the mesh transformation.

Mesh Transform Matrix

The mesh can be transformed using an [affine transform \(Wikipedia\)](#). Here the upper left 3 x 3 matrix describes a rotation, reflection, scaling or shear (or any combination of) and the 4th column a translation. This 4 x 4 matrix must be supplied as a 4 x 4 numpy array. Any number of transforms can be concatenated together to give the final position. Helper functions for rotations, translations and scalings are provided in `zutil.transform`. An example is given below:

```
import zutil.transform

A2B = zutil.transform.rotate([0.0, 1.0, 0.0], 10.0)
# If a matrix is passed as the last parameter to zutil.transform.* then the transform
→ is concatenated to it.
B2C = zutil.transform.scale([0.1, 0.1, 0.1], A2B)
C2D = zutil.transform.translate([0.0, 0.0, 0.0], [-1.0, 0.0, 0.0], B2C)

"mesh transform matrix": C2D
```

When using the `zutil.transform` helper functions transforms are applied in the order in which the user calls the functions. Rotations are considered using the same conventions as `pytransform3d` and are interpreted as active and applied using the pre-multiplication convention. For more complex transformations `pytransform3d` provides a comprehensive collection of python functions and can be easily interfaced with zCFD by simply passing the resulting transformation matrix to the solver.

Mesh Quality Remediation

Keyword	Required	Default	Valid values
'mesh quality remediation angle threshold'	No	'not set'	0 - 180

zCFD has the ability to detect poor quality cells in the mesh and fix them as first order in space. A poor quality cell is defined as one which has a face where the angle between the cell centre to cell centre vector and the face centre to cell centre vector is greater than that set using the `'mesh quality remediation angle threshold'` key. When convergence issues are encountered due to mesh quality setting the angle threshold to around 75 degrees initially may allow the solver to run on the mesh. Ideally the mesh should be improved so the solution can be fully second order over the entire domain.

Partitioner

Keyword	Required	Default	Valid values
'partitioner'	No	'metis'	['metis']. The name of the partitioner to use.

The `'metis'` partitioner is used to split the computational mesh up so that the job can be run in parallel. Other partitioners will be added in future code releases

Restart

Keyword	Required	Default	Valid values
'restart'	No	False	True/False
'restart casename'	No		Optionally supply the name of a case to restart from that case, if not supplied then the current casename will be used.
'restart ignore history'	No	False	True/False: True to ignore the cycle history from restart file and begin the solve as specified in current control file.
'interpolate restart'	No	False	True/False: True to interpolate restart results from a different mesh.
'restart meshname'	No	False	The name of the mesh to interpolate the restart from.
'solution smooth cycles'	No	0	Number of Laplace smoothing cycles to smooth initial mapped solution

Restart allows you to load a solution from a previous run and continue the solver from that point. By default the solver will look for a `<casename>_results.h5` file to load the restart, this can be overridden with the `'restart`

casename' parameter. The cycle history from the restart case can be ignored through the 'restart ignore history' option. To begin the current simulation using the <casename>_results.h5 specified in the current control dictionary but ignore the previous cycle history set this option to True.

The default restart assumes that the same mesh is used. Alternatively, a solution from another mesh can be mapped on to a new mesh using the 'interpolate restart' parameter.

Example usage:

```
# Restart from previous solution
'restart': True,
# Load solution from case name 'my_case'
'restart casename': 'my_case',
'restart ignore history': False,
```

```
# Restart from previous solution on a different mesh
"interpolate restart": True,
# Interpolate restart from "different_mesh.h5"
'restart meshname': "different_mesh",
# Do not smooth initial solution
"solution smooth cycles": 0,
```

Advanced Restart

It is possible to restart the SA-neg solver from results generated using the Menter SST solver and vice versa, however by default the turbulence field(s) are reset to zero. An approximate initial solution for the SA-neg model can be generated from Menter-SST results by adding the key

```
# Generate approximate initial field for SA-neg
'approximate sa from sst results': True,
```

Safe Mode

Keyword	Re-quired	Default	Valid values
'safe'	No	False	True/False

Safe mode turns on extra checks and provides diagnosis in the case of solver stability issues

Example usage:

```
# Enable safe mode
'safe': True,
```

1.5.2 Boundary Conditions

Boundary condition properties are defined using consecutively numbered blocks.

```
'BC_1' : {...},
'BC_2' : {...},
```

zCFD supports the following boundary condition types:

BC Type	Description
<i>Wall</i>	Wall boundaries
<i>Farfield</i>	Farfield boundaries with automatic inflow/outflow detection
<i>Inflow</i>	Pressure or massflow inflow boundaries
<i>Outflow</i>	Pressure or massflow outflow boundaries
<i>Symmetry</i>	Mirror boundary condition
<i>Overset</i>	The boundary of a mesh to be overset on a background mesh
<i>Periodic</i>	Repeating boundary condition, with flow from one periodic boundary mapped to the other.

“ref” and “zone”

Boundary conditions can be mapped to the mesh in two ways, depending on the mesh format used. Some mesh formats (for example Fluent) will have boundaries tagged with an integer (wall = 3, etc). These can be referenced directly using the “**ref**” keyword in your boundary condition definition. Alternatively, the mesh format may contain explicitly numbered zones (which can be determined by inspecting the mesh). In this case, the user can specify the list of zone numbers for each boundary condition using the “**zone**” keyword.

For example to apply BC_1 to boundaries tagged with value 3:

```
..
'BC_1' : {
    'ref' : 3,
    ..
}
..
```

Or to apply BC_1 to boundaries to zones with IDs 0,1,2 & 3:

```
..
'BC_1' : {
    'zone' : [0,1,2,3],
    ..
}
..
```

Note

If a ‘**zone**’ entry is provided it will override the IDs specified in ‘**refs**’

Wall

Wall boundaries in zCFD can be either slip walls, no-slip walls, or use automatic wall functions. No-slip walls are appropriate when the mesh is able to fully resolve the boundary layer (i.e $y^+ \leq 1$) otherwise automatic wall functions should be used. This behaviour is chosen by setting 'kind' in the wall specification below. Optionally it is possible to set wall velocity, roughness and temperature.

'type' allows you to choose between a standard 'wall' definition or 'immersed wall' boundaries. Immersed wall boundaries are *only* supported with meshes created by the using *zM3* mesh generator. The *zM3* mesh generator will determine vectors to represent the underlying geometry within the 3D Cartesian mesh. It will also generate additional information such as locations where data is to be sampled in order to define conditions at the geometry surface, and the subsequent halo boundary values.

Note

Immersed wall boundaries supports 'type' of 'slip', 'noslip' or 'wallfunction'.

If 'slip' conditions are chosen, there will be zero momentum normal to the underlying geometry.

If 'noslip' conditions are chosen, any values computed near the wall will linearly extrapolated from the donor (sample) point location associated with that point. This can potentially cause sensitivity and early flow separation in strong pressure gradients. Again, this can be alleviated to some extent with mesh refinement, however, this is associated with additional computational cost.

If 'wallfunction' conditions are chosen, any values computed near the wall will be based on the Musker wall model, which closely represents the flow along a flat plate in zero pressure gradient. As such, there are fundamental limitations on the accuracy of this model with highly curved surfaces and strong pressure gradients. This can be alleviated to some extent with mesh refinement, however, this is associated with additional computational cost.

Keyword	Re-quired	Default	Valid values	Description
'ref'	Yes		Integer	Mesh reference defined by this boundary condition
'zone'	No		List of integers	Specifies list of mesh zones defined by this boundary condition
'type'	No		'wall' or 'immersed wall'	Specifies a solid wall boundary which defaults to adiabatic unless a temperature is specified
'kind'	Yes		'slip', 'noslip', 'wallfunction'	Specifies the type of wall boundary condition. Slip - zero viscosity wall boundary. noslip - viscous wall with $y^+ \sim 1$ mesh resolution, wallfunction - viscous wall with automatic handling of mesh resolution between $y^+ \sim 1$ to $y^+ > 100$
'immersed normal type'	No	'STL'	'STL' or 'immersed boundary vector'	For 'immersed wall' types. Specifies how the geometry unit normals are specified (from the STL directly or approximated by the vector from the face centre to the nearest surface point)
'roughness'	No		See <i>roughness</i>	Specifies the surface roughness. If not specified the wall is specified as perfectly smooth. This requires the wall boundary condition kind to be set to wallfunction .
'v'	No		See <i>velocity</i>	Wall velocity specification.
'temperature'	No		See <i>temperature</i>	Specifies the wall temperature for an isothermal wall. If not specified the wall is treated as adiabatic

Example Wall BC with roughness and temperature set:

```
'BC_1' : {
  'ref' : 3,
  'type' : 'wall',
  'kind' : 'slip',
  'roughness' : {
    'type' : 'height',
    'scalar' : 0.001
  },
  'temperature' : {
    # Temperature in Kelvin
    'scalar' : 280.0,
  },
},
```

Example Immersed Boundary Wall BC:

```
'BC_1' : {
  'ref' : 3,
  'type' : 'immersed wall',
  'kind' : 'wallfunction',
  'immersed normal type' : 'STL',
},
```

Roughness

Keyword	Re-quired	Default	Valid values	Description
'type'	No		'height' or 'length'	Specify how roughness is being specified.
'scalar'	No		Positive float	Specify the value of roughness length or height in mesh units
'field'	No		Valid filename	Specify the name of a file that defines a roughness field. This file needs to contain a node array called Roughness that is used to set the value by finding the nearest point to the mesh location.

Roughness can be specified as either a 'height' or 'length'.

Roughness **length** is defined as the height at which the mean velocity profile of the flow is zero. In other words, at this distant above the surface, the flow is considered to be effectively smooth, and the velocity distribution approaches a logarithmic law.

Roughness **height** refers to the average height or magnitude of surface roughness elements on a solid boundary. It represents the scale of irregularities or protrusions on the surface, which disrupt the smooth flow and create additional drag or turbulence. Examples of roughness elements include bumps, ridges, or rough surface textures.

This value can be given as a single **scaler** value or a **field** file can be provided. This should be a VTP file containing a node array called "Roughness". The roughness at each boundary face is then set by finding the nearest point to the face centre on the supplied VTK file with the roughness value looked up in a node based scalar array called 'Roughness'

Velocity

The velocity keywords are used to apply a surface velocity, this is used to model cases with surfaces in relative motion. e.g. a car moving over a road surface or rotating tyre surface. The wall boundary condition supports either a **linear** velocity or a **rotating** one

The options for the '**linear**' dictionary are:

Keyword	Re-quired	Default	Valid values	Description
'vector'	Yes		[x, y, z]: vector of numbers	Sets the velocity vector for the translation motion of the surface.
'mach'	No		Number	Overrides the magnitude of the translation velocity vector

The options for the '**rotating**' dictionary are:

Keyword	Re-quired	Default	Valid values	Description
'axis'	Yes		[x, y, z]: vector of numbers	Sets the axis of rotation
'origin'	Yes		[x, y, z]: vector of numbers	Sets the origin of the rotation axis
'omega'	Yes		Number	Sets the rotational velocity of the rotation in radians per second

Example Linear Velocity Boundary Wall BC:

```
'BC_1': {
  'zone': [1],
  'type': 'wall',
  'kind': "noslip",
  'v': {
    'linear': {
      'vector': [1.0,0,0],
      'mach': 0.5, # optional override to vector magnitude
    },
  },
},
```

Example Rotating Velocity Boundary Wall BC:

```
'BC_1': {
  'zone': [7],
  'type': 'wall',
  'kind': "wallfunction",
  'v': {
    'rotating': {
      'axis': [-1,0,0],
      'origin': [0,0,0],
      'omega': 10, # radians per second
    },
  },
},
```

Temperature

The temperature keywords are used to apply a surface temperature. A scalar temperature can be applied to the whole boundary or a VTP file provided containing a temperature **'field'**. When using a **'field'** The temperature at each boundary face is set by finding the nearest point to the face centre on the supplied VTP file with the temperature value looked up in a node based scalar array called 'Temperature'

The options for the **'temperature'** dictionary are:

Keyword	Re-quired	Default	Valid values	Description
'scalar'	Yes		number	Specify the value of wall temperature in Kelvin
'field'	No		Valid filename	Specify the name of a file that defines a temperature field. This file needs to contain a node array called <i>Temperature</i> that is used to set the value by finding the nearest point to the mesh location for an isothermal wall.

Farfield

Farfield boundary conditions are typically used for external flow simulations and automatically switch for inflows or outflows. This boundary condition cannot be used with the incompressible solver. The farfield boundary automatically determines whether the flow is locally an inflow or an outflow by solving a Riemann equation. The conditions on the farfield boundary are set by referring to an ' IC_ ' block. In addition to this an atmospheric boundary layer profile or a turbulence profile may be set.

Keyword	Re-quired	Default	Valid values	Description
'ref'	Yes		Integer	Mesh reference defined by this boundary condition
'zone'	No		List of integers	Specifies list of mesh zones defined by this boundary condition
'type'	Yes		'farfield'	This sets the type of boundary condition to be associated with the zones.
'kind'	Yes	'riemann'	'riemann', 'pressure', 'supersonic' or 'preconditioned'	<p>This sets the specific model used for the farfield boundary condition:</p> <ul style="list-style-type: none"> <i>riemann</i> uses riemann invariants to provide a non reflecting inflow with a pressure outflow. <i>pressure</i> uses a pressure boundary condition for both inflow (downstream pressure) and outflow (user specified pressure). <i>supersonic</i> uses a supersonic boundary conditions by using upstream conditions for both inflow and outflow. <i>preconditioned</i> uses a preconditioned variant of the riemann boundary condition.
'condition'	Yes		String reference to IC	Set the reference flow conditions block that relates to these boundaries, see <i>IC_*</i> .

Example boundary condition block for a farfield boundary:

```
'BC_2' : {
    # Zone type tag
    'ref' : 9,
    # Optional: Specific zone boundary condition override
    'zone' : [0,1,2,3],
    # Required: Boundary condition type
    'type' : 'farfield',
    # Required: Kind of farfield options (riemann, pressure or supersonic)
    'kind' : 'riemann',
    # Required: Farfield conditions
    'condition' : 'IC_1',
    # Optional: Atmospheric Boundary Layer
},
```

Inflow

zCFD can specify two kinds of inflow boundary condition: pressure or massflow, selected using the 'kind' key. When using the pressure inflow the boundary condition is specified by a total pressure ratio and a total temperature ratio that needs to be defined by the condition this refers to. When using the massflow condition a total temperature ratio and mass flow ratio or a mass flow rate is required. Note the mass flow ratio is defined relative to the condition set in the 'reference' key. By default the flow direction is normal to the boundary but either a single vector or a python function can be used to specify the inflow normal vector of each face on

the surface.

Note

The massflow rate needs to be specified in kg/s and can only be used if the mesh is in metres. Massflow ratio is nondimensional where A_{in} is defined in mesh units. Given $massflowratio = \rho_{in} U_{in} A_{in} / (\rho_{ref} U_{ref})$

Keyword	Re-quired	Default	Valid values	Description
'ref'	Yes		Integer	Mesh reference defined by this boundary condition
'zone'	No		List of integers	Specifies list of mesh zones defined by this boundary condition
'type'	Yes		'inflow'	This sets the type of boundary condition to be associated with the zones.
'kind'	Yes	'default'	'default' or 'mass-flow'	<p>This sets the how the user wants to specify the inflow boundary condition:</p> <ul style="list-style-type: none"> <i>default.</i> Pressure inflow. Velocity and density are calculated from the user provided total pressure ratio and total temperature ratio set in the reference condition. The direction of the velocity vector uses the surface normal but a specific direction can also be provided by the user. Local static pressure is used to compute a local mach number from the total pressure ratio. If the user specifies a mach number this is used to set the static pressure from the total pressure ratio. <i>massflow</i> The velocity is set from the massflow set in the reference condition.
'condition'	Yes		String reference to IC	Set the reference flow conditions block that relates to these boundaries, see <i>IC_*</i> .

Example boundary condition for setting up a **pressure** inflow condition based on flow conditions defined in *IC_2*:

```
'BC_3' : {
    'ref' : 4,
    'type' : 'inflow',
    'kind' : 'default',
    'condition' : 'IC_2',
  },
```

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```

'IC_1' : {
  'temperature' : 293.0,
  'pressure' : 101325.0,
  'V': {
    'vector' : [1.0,0.0,0.0],
    'Mach' : 0.20,
  },
  'Reynolds No' : 1.0e6,
  'Reference Length' : 1.0,
  'turbulence intensity' : 0.1,
  'eddy viscosity ratio' : 1.0,
},
'IC_2' : {
  'reference' : 'IC_1',
  'total temperature ratio' : 1.0,
  'total pressure ratio' : 1.0,
  # Optional - specify mach number to set
  # static pressure at inflow from total pressure
  'mach' : 0.1,
},
},

```

Example boundary condition for setting up a **massflow** inflow condition based on flow conditions defined in *IC_2*:

```

'BC_3' : {
  'ref' : 4,
  'type' : 'inflow',
  'kind' : 'massflow',
  'condition' : 'IC_2',
},
'IC_1' : {
  'temperature' : 293.0,
  'pressure' : 101325.0,
  'V': {
    'vector' : [1.0,0.0,0.0],
    'Mach' : 0.20,
  },
  'Reynolds No' : 1.0e6,
  'Reference Length' : 1.0,
  'turbulence intensity' : 0.1,
  'eddy viscosity ratio' : 1.0,
},
'IC_2' : {
  'reference' : 'IC_1',
  'total temperature ratio' : 1.0,
  'mass flow rate' : 10.0,
},
},

```

Outflow

Pressure or massflow outflow boundaries are specified in a similar manner to the *Inflow* boundary. They can be of 'kind' 'pressure', 'radial pressure gradient' or 'massflow'. When the boundary condition 'kind' is either 'pressure' or 'radial pressure gradient', the 'IC_' conditions it refers to must set a static pressure ratio. When the boundary condition 'kind' is 'massflow', a mass flow ratio or mass flow rate must be set in the 'IC_' conditions. Note the mass flow ratio is defined relative to the condition set in the 'reference' key.

Note

The massflow rate needs to be specified in kg/s and can only be used if the mesh is in metres. Massflow ratio is nondimensional where A_{out} is defined in mesh units. Given $massflowratio = \rho_{out}U_{out}A_{out}/(\rho_{ref}U_{ref})$

Keyword	Re-quired	Default	Valid values	Description
'ref'	Yes		Integer	Mesh reference defined by this boundary condition
'zone'	No		List of integers	Specifies list of mesh zones defined by this boundary condition
'type'	Yes		'outflow'	This sets the type of boundary condition to be associated with the zones.
'kind'	Yes		'pressure' or 'massflow' or 'radial pressure gradient'	This sets how the user wants to specify the outflow conditions: <ul style="list-style-type: none"> <i>pressure</i> Sets the pressure at the outflow using the user specified static pressure ratio set in the reference condition. <i>massflow</i> Scales the local velocity so that the total integrated massflow across all the zones meets the user specified value.
'condition'	Yes		String reference to IC	Set the reference flow conditions block that relates to these boundaries, see <i>IC_*</i> .
'reference radius'	Yes		Number	

```
'BC_4' : {
  # Zone type tag
  'ref' : 5,
  # Optional: Specific zone boundary condition override
  'zone' : [0,1,2,3],
  # Boundary condition type
  'type' : 'outflow',
  # Kind of outflow 'pressure', 'massflow' or 'radial pressure gradient'
  'kind' : 'pressure',
  # Required only when using 'radial pressure gradient'
  # Radius at which the static pressure ratio is defined
  'reference radius' : 1.0,
  # Outflow conditions
  'condition' : 'IC_2',
},
```

Symmetry

Keyword	Re-quired	Default	Valid values	Description
'ref'	Yes		Integer	Mesh reference defined by this boundary condition
'zone'	No		List of integers	Specifies list of mesh zones defined by this boundary condition
'type'	Yes		'symmetry'	This sets the type of boundary condition to be associated with the zones.

Example symmetry boundary condition:

```
'BC_5' : {
    'ref' : 7,
    'type' : 'symmetry',
},
```

Periodic

This boundary condition needs to be specified in pairs with opposing transformations. The transforms specified should map each zone onto each other.

Note

Each periodic boundary needs to provide the correct vector to the opposite matching boundary.

Keyword	Re-quired	Default	Valid values	Description
'ref'	Yes		Integer	Mesh reference defined by this boundary condition
'zone'	No		List of integers	Specifies list of mesh zones defined by this boundary condition
'type'	Yes		'periodic'	This sets the type of boundary condition to be associated with the zones.
'kind'	Yes		'rotated' or 'linear' dictionary (see below)	The definition of the periodic transformations, can either be a 'rotated' or 'linear' dictionary

The options for the '**linear**' dictionary are:

Keyword	Re-quired	Default	Valid values	Description
'vector'	Yes		[x, y, z]: vector of numbers	Defines the translation vector to map this zone onto the matching periodic zone

Example linear periodic boundary condition:

```
'BC_6' : {
    'zone' : [1],
```

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```

    'type' : 'periodic',
    'kind' : {
        # Linear periodic settings
        'linear' : {
            'vector' : [1.0,0.0,0.0],
        },
    },
},

```

The options for the **'rotated'** dictionary are:

Keyword	Re-quired	Default	Valid values	Description
'axis'	Yes		[x, y, z]: vector of numbers	Defines the axis of rotation used to map this boundary onto the matching periodic zone
'origin'	Yes		[x, y, z]: vector of numbers	Defines the origin of the axis of rotation
'theta'	Yes		Number	Defines the angle of rotation about the axis (in radians)

Example rotated periodic boundary condition:

```

'BC_6' : {
    'zone' : [1],
    'type' : 'periodic',
    'kind' : {
        # Rotated periodic settings
        'rotated' : {
            'theta' : math.radians(120.0),
            'axis' : [1.0,0.0,0.0],
            'origin' : [-1.0,0.0,0.0],
        },
    },
}

```

Overset

The overset boundary condition should be applied to the boundaries of a mesh to be overset on top of a larger background mesh.

Keyword	Re-quired	Default	Valid values	Description
'ref'	Yes		Integer	Mesh reference defined by this boundary condition
'zone'	No		List of integers	Specifies list of mesh zones defined by this boundary condition
'type'	Yes		'overset'	This sets the type of boundary condition to be associated with the zones.

Example overset boundary condition:

```
'BC_7' : {
    'zone': [1,2,3,4],
    'type' : 'overset',
},
```

1.5.3 Time Marching

zCFD is capable of performing both steady-state and time dependent simulations. Steady-state solutions are marched in pseudo time towards convergence. Time dependent simulations can be either globally time-stepped or use local pseudo time-stepping within a dual time-stepping iteration in physical time. The 'time marching' dictionary controls the selection of these schemes. Major options are what CFL number to use, whether explicit or implicit time-stepping is used and whether the simulation is time dependent.

```
parameters = {
    ...
    "time marching": {
        "cycles": 5000,
        "unsteady": {...},
        "scheme": {...},
        'cfl': 30.0,
        "multigrid": 3,
        "multigrid cycles": 20000,
        "moving mesh": False,
    },
    ...
}
```

Cycles

The total number of pseudo time-steps to use in a *steady-state* simulation, or the number of pseudo time-steps to use in each real time-step of an *unsteady* time-dependent simulation

Example usage:

```
# A good starting value for most explicit, steady state cases. Implicit simulations
- can use a higher CFL and therefore require fewer cycles - around 100 - 500 cycles
- is a good starting point for an implicit steady state case.
'cycles' : 5000,
```

CFL Control

The Courant-Friedrichs-Lewy (CFL) number controls the local pseudo time-step that the solver uses to reach a converged solution. The larger the CFL number, the faster the solver will run but the less stable it will be. The CFL dictionary keys are only valid when using dual time-stepping.

Keyword	Re-quired	Default	Valid values
'cfl'	Yes	0	Any positive floating point number.
'cfl transport'	No	–	Any positive floating point number.
'cfl ramp'	No	–	Dictionary containing 'initial' and 'growth' - respectively the starting CFL number and the growth rate applied as a multiplier each successive time step until the CFL number is reached.
'ramp func'	No	–	Instead of the 'cfl ramp' parameter the user can specify a <i>ramp function</i> .
'cfl coarse'	No	Current CFL number	Any positive floating point number.
'cfl viscous factor'	Yes	1	Any positive floating point number.

cfl

Sets the CFL number used in the mass, momentum and energy equations.

Example usage:

```
# Typical value used for a RANS simulation using explicit time marching
'cfl' : 1
```

```
# Typical value used for a RANS simulations using implicit time marching
'cfl' : 30
```

Note

Besides mesh quality, CFL is the most important parameter affecting simulation stability. If you find your simulation does not converge, consider reducing CFL

cfl transport

Sets the maximum CFL number used to update the turbulent transport equations (for example k and ω).

```
# Use cfl transport to promote solver stability
'cfl' : 30,
'cfl transport': 20
```

Note

If you find your simulation does not converge and reports high turbulence equation residuals which increase with successive cycles, consider setting this to a value lower than 'cfl'

cfl ramp

This allows a relatively large target CFL number to be specified, but start the simulation using a smaller one to provide stability as large non-physical transients are eliminated from the solution.

Starting a simulation with a large CFL number can cause instability to crash the solver. A more gentle start will reduce the impact of non-physical transients.

```
# Start cfl at 0.1 and grow at a rate 1.1, reaching the target cfl of 30 in 26 steps
'cfl' : 30,
'cfl ramp': {
  'initial': 0.1,
  'growth': 1.1
}
```

cfl coarse

For simulations with multigrid acceleration, the **'cfl coarse'** number is used as a CFL condition on the coarse meshes. For such cases the **'cfl'** number is still applied to the finest mesh.

This only applies to explicit finite volume solutions.

```
# The quality of agglomerated (multigrid) coarse meshes is typically less than the
- quality of the primary (fine) mesh and so a lower CFL number may be required for
- numerical stability.
'cfl' : 1.0,
'cfl coarse': 0.5
```

cfl viscous factor

Factor applied to the diffusive (viscous) time step when applying the CFL condition. As viscous effects are rarely the cause of solver instability, the contribution of the viscous terms to the time step evaluation may be reduced by setting **'cfl viscous factor'** to a number less than 1.

```
# For the low Reynolds number cylinder case, viscous effects are dominant but do not
- contribute to instability.
# The value of 1e-6 effectively discounts viscosity in the determination of the time
- step when applying the CFL condition.
"cfl": 200,
"cfl viscous factor": 1.0E-6,
"cfl ramp factor": {"initial": 0.1, "growth": 1.05},
```

Solver scheme

There are two different time marching schemes available in zCFD: multistage explicit and euler implicit scheme. These can be used for both steady and unsteady (using global or dual time-stepping) simulations. Global time-stepping requires no preconditioning and excludes some of the multistage RK schemes.

Keyword	Required	Default	Valid values	Description
'name'	Yes	"runge kutta"	"euler" "runge kutta" "implicit euler"	Name of scheme
'stage'	No	"rk third order tvd"	1 4 5 'rk third order tvd'	("runge kutta" only) Number of RK stages
'kind'	No	-	'local timestepping' 'global timestepping'	Timestepping mode

Note

The Euler scheme has a single stage and is the safest option for new or problematic cases.

name

The solution is integrated in time (solved) using an integration scheme that can be either explicit (variables driving the change are evaluated at the previous step) or implicit (some or all of the variables driving the change are evaluated at the current step). **'euler'** or **'runge kutta'** are the explicit schemes and **'implicit euler'** is the implicit option.

A larger time step can be taken using the implicit scheme, as the method is more stable than an explicit scheme.

Note

The trade off in using implicit time integration is the increase in memory requirement, typically 3-5 times more than for an explicit scheme.

stage

The number of Runge-Kutta stages in each step of the integration scheme affects the order of temporal convergence, and affects the maximum CFL that can be used.

Note

For most of the test cases where Runge-Kutta integration is used, 5 stages are applied. This is a typical industry standard and has been shown to be robust for most test cases.

kind

Global time stepping uses the same time step in each cell for the integration, whereas local time stepping calculates and uses the time step in each cell as determined by the local flow conditions and the prescribed CFL number. In cases where there are very small cells. it would be impractical to use global timestepping as all the cells would have to march at the pace of the slowest.

Note

While global timestepping restricts all cells to the smallest timestep and should only be used for unsteady simulations.

Unsteady

The Unsteady dictionary controls the simulation time and can be used to set up both Steady and Unsteady cases.

Keyword	Required	Default	Valid values	Description
'total time'	Yes	–	Positive float	Total time to simulate
'time step'	Yes	–	Positive float	Physical time step for the simulation
'order'	Yes	"second"	"first" "second" 1 2	(Unsteady only) Order of time integration.
'start'	No	–	Positive integer	(Unsteady only) For unsteady simulations, how many steady-state timesteps to run to initialise solution.

Running steady state

For steady-state simulations, **'total time'** should be set equal to the **'time step'** value. The solver will then automatically run a steady-state simulation.

Example usage:

```
# Run an steady state simulation
'time marching' : {
    ...
    "unsteady": {
        "total time": 1.0,
        "time step": 1.0,
    },
    ...
}
```

Running unsteady

If the **'time step'** value is less than the **'total time'** value, then an unsteady simulation is created.

Time integration for unsteady simulations is based on the solution at the current time step and the contribution of the solution in previous time steps, represented by a Backward Difference Formula. Dual time-stepping is used to update the current solution with data from previous time steps. **'order'** controls the order of the Dual time-stepping.

'start' provides the option of initialising an unsteady simulation with a number of steady-state pseudo timesteps.

Example usage:

The unsteady laminar cylinder test case sheds a vortex street with a specific Strouhal number. We want to run the simulation for 1.7 seconds to allow the oscillation to begin and establish a well-formed pattern. We set the time step to a small enough value to capture the unsteady shedding phenomenon.

```
# Run an unsteady simulation for 1.7 seconds with a time step of 0.002 seconds
'time marching' : {
  ...
  "unsteady": {
    "total time": 1.7,
    "time step": 0.002,
    "order": "second",
    "start": 0
  },
  ...
}
```

The example below uses a relatively large time step and maintains accuracy with a second order integration scheme. The case starts with 2000 pseudo-timesteps before starting the unsteady simulation.

```
# Run an unsteady simulation for 1.7 seconds with a time step of 0.002 seconds
'time marching' : {
  ...
  "unsteady": {
    "total time": 0.06,
    "time step": 2.0e-5,
    "order": "second",
    "start": 2000
  },
  ...
}
```

Multigrid

Keyword	Re-quired	Default	Valid values
'multigrid'	No	-	Any positive integer.
'multigrid cycles'	No	-	Any positive integer.

To accelerate an explicit finite volume solution, coarse meshes are generated from the original (fine) mesh by agglomerating or combining cells together to create larger cells. The **'multigrid'** value sets the number of successive times to apply this operation, each iteration resulting in a coarser mesh with fewer cells. By solving on the hierarchy of coarser meshes as well as the fine mesh, information is moved faster in the flow domain and a converged solution is reached more efficiently. The multigrid scheme is designed so that the acceleration does not (in theory) change the result that would be obtained just by solving on the finest mesh alone, though in practice the use of multigrid does ultimately stall convergence on most meshes.

Use multigrid acceleration for a specified number of **'multigrid cycles'** and then revert to the finest mesh only. This is to make use of the more efficient scheme at the start, and avoid convergence stall due to multigrid at the end of a solution process.

Example usage:

```
# 3 levels of multigrid is sufficient in most cases to reduce the number of cycles,
# -required by an order of magnitude.
# If this causes instability, a reduction to 2 may solve the problem.
'time marching' : {
  ...
  'multigrid': 3,
  ...
}
```

```
# After 20000 explicit cycles, multigrid stall prevents convergence to the correct
-drag value.
# By turning it off, the correct value is obtained on the finest mesh.
'time marching' : {
    ...
    'multigrid': 3,
    'multigrid cycles' 20000,
    ...
}
```

Note

Multigrid only applies to explicit finite volume solutions.

Moving Mesh

Keyword	Re-quired	Default	Valid values
'moving mesh'	No	False	True False

In any case where the mesh (or a fluid zone within the mesh) is moving (translation or rotation) the simulation can be performed in either the frame of reference of the mesh or in a fixed coordinate system. For simulations where there is no relative movement of interest, **'moving mesh'** may be set to False. For simulations where there is relative movement, setting **'moving mesh'** to True will force a recalculation of the physical location of the mesh, including the recalculation of any overset mappings.

1.5.4 Linear Solver Settings

There are several situations where the options selected in zCFD require the solution of a linear system. These are:

- When the *Time Marching* scheme is set to euler implicit.
- When RBFs are used for mesh motion.
- When the incompressible solver is selected.

When running on CPUs zCFD uses **Petsc** linear solver library and when running on NVidia GPUs zCFD uses the **AMGX** linear solver library. Both libraries offer a wide array of solver and preconditioner choices and altering the settings can have a significant impact on the performance and convergence of the solver. Options can be passed to Petsc via the control dictionary and AMGX options are set using a json file which is read at runtime.

Petsc

Details of the available options for the Petsc KSP linear system solvers used by zCFD are given [here](#). these options can be passed through to Petsc via the zCFD control dictionary using the "linear solver options" key. The default values are given below:

```
"linear solver options": {"flow": { "-ksp_type": "fgmres",
                                   "-ksp_rtol": "1.0e-3",
                                   "-ksp_monitor": "",
                                   "-ksp_converged_reason": "" },
                          "turbulence": { "-ksp_type": "fgmres",
                                           "-ksp_rtol": "1.0e-5",
                                           "-ksp_monitor": "",
                                           "-ksp_converged_reason": "" },
```

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```

    "rbf": { "-ksp_type": "fgmres",
            "-ksp_rtol": "1.0e-5",
            "-ksp_monitor": "" }
  }

```

Settings are provided for the mean flow, turbulence and RBF linear systems. Most of the settings detailed in the [Petsc documentation](#) can be passed through by adding them as key, value pairs to the appropriate dictionary. Where an option doesn't take a value an empty string needs to be provided.

The [Hypre](#) library of algebraic multigrid methods is available via [Petsc PCHYPRE](#) and the associated settings can be supplied via the "linear solver options" dictionary. Using Hypre's boomeramg package as a preconditioner has shown good performance with the incompressible solver:

```

"linear solver options": {"flow": { "-ksp_type": "fgmres",
                                   "-ksp_rtol": "1.0e-3",
                                   "-ksp_monitor": "",
                                   "-ksp_converged_reason": "",
                                   "-pc_type": "hypre",
                                   "-pc_hypre_type": "boomeramg"},
  ...

```

Further Hypre options are detailed in the [Petsc PCHYPRE](#) documentation.

AMGX

The AMGX settings for the mean flow, turbulence and RBF linear systems can be found in ZCFD_HOME/amgx.json, ZCFD_HOME/turbamgx.json and ZCFD_HOME/RBF_amgx.json. The mean flow settings are shown below:

```

"config_version": 2,
"determinism_flag": 1,
"solver": {
  "preconditioner": {
    "error_scaling": 0,
    "print_grid_stats": 0,
    "max_uncolored_percentage": 0.05,
    "algorithm": "AGGREGATION",
    "solver": "AMG",
    "smoother": "MULTICOLOR_GS",
    "presweeps": 0,
    "selector": "SIZE_8",
    "coarse_solver": "NOSOLVER",
    "max_iters": 1,
    "postsweeps": 3,
    "min_coarse_rows": 32,
    "relaxation_factor": 0.75,
    "scope": "amg",
    "max_levels": 40,
    "matrix_coloring_scheme": "PARALLEL_GREEDY",
    "cycle": "V"
  },
  "use_scalar_norm": 1,
  "solver": "FGMRES",
  "print_solve_stats": 1,
  "obtain_timings": 1,
  "max_iters": 10,
  "monitor_residual": 1,

```

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```

"gmres_n_restart": 5,
"convergence": "RELATIVE_INI_CORE",
"scope": "main",
"tolerance": 1e-3,
"norm": "L2"
}

```

In general these settings provide good performance for most cases. If issues are encountered converging the linear system reducing the “tolerance” may help. Otherwise altering the multigrid aggregation selection algorithm “selector”: “SIZE_8” to “SIZE_4” or “SIZE_2” will build smaller aggregates and hence increase the number of coarse levels - improving convergence at the expense of memory use. Increasing the number of “gmres_n_restart” may also improve convergence at the expense of increased memory use.

There are too many AMGX options to detail here but example configurations for different solvers are given [here](#).

When running on NVidia GPUs and using AMGX there is only one option available in the “linear solver options” dictionary:

```
"linear solver options": {"double precision": False}
```

The “double precision” option controls whether the mean flow linear system is solved in single or double precision. Solving in single precision brings a reduction in memory use and a speed up to the solver. However, double precision may be required for more challenging cases.

1.5.5 Equations

Keyword	Re-quired	Default	Valid values
‘equations’	Yes	–	Any of equation sets detailed below.

The equations key selects the equation set to be solved.

The corresponding equation set options should also be defined in the control dictionary. The valid equation keys are shown in the table below.

Solver	Description	Com-pressible	Incom-pressible
Euler	Use the Euler flow equations in the simulation. These are compressible, inviscid flow equations.	<i>“euler”</i>	–
Viscous	Use the viscous flow equations. These are compressible, viscid flow equations which do not model turbulence.	<i>“viscous”</i>	<i>“incomp viscous”</i>
RANS	Use the RANS (Reynolds-Averaged Navier-Stokes) equations in the simulation. These are compressible, viscid flow equations with additional terms included to account for the effect of turbulence on the flow without the expense of simulating the turbulent flow structures themselves.	<i>“rans”</i>	<i>“incomp rans”</i>
LES	Use the Large Eddy Simulation (LES) equations.	<i>“les”</i>	<i>“incomp les”</i>

Example usage:

```

parameters = {
  ..
  # Use the euler equation set

```

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```
'equations' : 'euler',
# Define the inputs for the 'euler' equation set
'euler': {...}
..
}
```

Common Settings

The following parameters are common for all of the equation sets.

Keyword	Required	Default	Valid values
'order'	Yes	–	'first' 'second' 'euler_second'
'first order cycles'	No	–	Positive integer
'linear gradients'	No	False	True False
'leastsq gradients'	No	False	True False
'inviscid flux scheme'	Yes	"Roe"	"HLLC" "Rusanov" "Roe" "Roe low diss"
'reconstruction'	No	"muscl"	"muscl" "umuscl" "lpumuscl"
'entropy fix'	No	"0.0"	Float between 0.0 and 0.2
'roe low dissipation sensor'	No	–	"FD" "NTS" "DES" "NONE"
'roe dissipation sensor minimum'	No	–	Float between 0.05 and 1.0
'freeze limiter cycle'	No	–	Positive integer
'relax'	Yes (for incompressible equation set)	0.5	Positive float
'turbulence'	Yes (for 'les' or 'rans' equation set)	{}	See <i>"turbulence"</i>

order

Sets the order of the spatial discretisation. **'euler_second'** is second order for the flow variables and first order for the turbulence.

first order cycles

Specifies the number of cycles the solver will run with first order spatial discretisation. This can be used to improve stability at start up. If the solver is dual time stepping then the number of first order cycles is taken as the total number from the start of the simulation.

Example usage: Run 500 cycles first order.

```
parameters = {
..
'equations' : 'euler',
'euler': {
...
'first order cycles': 500,
...
}
..
}
```

linear gradients & leastsq gradients

By default zCFD uses a Weighted Green-Gauss gradient calculation. This can be switched to a standard Green-Gauss by setting **'linear gradients'** to True. Setting **'leastsq gradients'** to True will set the gradient calculation to Least Squares.

inviscid flux scheme

Picks the scheme to use for the inviscid flux. **HLLC** is good when running explicit, **Roe** is best for implicit and **Rusanov** is good for getting an implicit simulation going. The **Roe low diss** scheme can be used with LES or Hybrid RANS/LES

roe low dissipation sensor

The sensor used to decide whether to use (and by how much) the Roe low dissipation scheme.

Setting	Notes
'DES'	Uses the blending function from the selected DES model to turn on the Roe low dissipation scheme in LES regions
'NONE'	Uses the value set on 'roe dissipation sensor minimum' everywhere
'FD'	See Johnsen et al. JCP 229 (2010) pag. 1234
'NTS'	See Xiao et al. INT J HEAT FLUID FL 51 (2015) pag. 141 https://doi.org/10.1016/j.ijheatfluidflow.2014.10.007

roe dissipation sensor minimum

Sets the minimum value that the dissipation term in the Roe scheme is multiplied by when using the **'Roe low diss'** scheme. This allows you control the stability of the low diss scheme (smaller values reduce the dissipation and hence the stability of the scheme)

freeze limiter cycle

If set the values of the limiter used in the MUSCL reconstruction are frozen at the specified cycle. This can be useful in the latter stages of a simulation if noise from the limiter is causing the residual convergence to stall.

relax

The relaxation factor used on the flow equations in the incompressible solver. Increasing this will speed up convergence at the expense of stability and vice versa.

turbulence

The turbulence dictionary is required for the *"rans"* and *"les"* equations sets.

Euler

Compressible Euler flow is inviscid (no viscosity and hence no turbulence). The compressible Euler equations are appropriate when modelling flows where momentum significantly dominates viscosity - for example at very high speed. The computational mesh used for Euler flow does not need to resolve the flow detail in the boundary layer and hence will generally have far fewer cells than the corresponding viscous mesh would have.

As well as the *"common"* settings, the following settings are available:

Keyword	Required	Default	Valid values	Description
'precondition'	Yes	False	True False	Use low speed mach preconditioner

Example usage:

```
parameters = {
  ..
  # Use the euler equation set
  'equations' : 'euler',
  'euler' : {
    'order' : 'second',
    'first order cycles': 100,
    # Cycle on which to freeze the limiter values
    'freeze limiter cycle': 500,
    # Use low speed mach preconditioner
    'precondition' : True,
    'Inviscid Flux Scheme': 'HLLC',
  },
}
```

Viscous

The viscous (laminar) equations model flow that is viscous but not turbulent. The **Reynolds number** of a flow regime determines whether or not the flow will be turbulent.

The computational mesh for a viscous flow has to resolve the boundary layer so will generally be larger than that used for an Euler simulation. A viscous simulation will run faster than a RANS simulation using the same mesh since fewer equations are being modelled.

As well as the “*common*” settings, the following settings are available:

Keyword	Required	Default	Valid values	Description
'precondition'	Yes	False	True False	Use low speed mach preconditioner

Example usage:

```
parameters = {
  ..
  # Use the viscous equation set
  'equations' : 'viscous',
  'viscous' : {
    'order' : 'second',
    'first order cycles': 100,
    # Use low speed mach preconditioner
    'precondition' : True,
    'linear gradients' : False,
    'Inviscid Flux Scheme': 'HLLC',
  },
  ..
}
```

Incompressible Viscous

Incompressible viscous equations follow the same structure as the compressible viscous equations with the addition of several parameters to address numerical challenges related to the orthogonality of the mesh. Note that the **scheme** block is not required.

Keyword	Required	Default	Valid values	Description
'relax'	Yes	0.5	Positive float	The relaxation factor used on the flow equations in the incompressible solver.
'correction'	Yes	'over relaxed'	'none' 'orthogonal' 'minimum' 'over relaxed'	Selects the type of non-orthogonal correction to apply to the flow equations.
'correction limiter'	Yes	0.5	Float between 0.0 and 1.0	Sets the limiter for the non-orthogonal correction. 1.0 applies the full correction, 0.0 turns off the correction.
'gradient limiter type'	Yes	'cell md'	'cell md' 'cell'	Selects the type of gradient limiter to apply to the flow equations. cell_md is more robust on highly non-orthogonal meshes. cell is less dissipative.
'gradient limiter'	Yes	0.5	Float between 0.0 and 1.0	Sets the coefficient for the gradient limiter. 1.0 is the most dissipative, 0.0 turns off the limiter.
'max second order non orthogonal angle'	Yes	90.0	Float between 0.0 and 90.0	Sets the maximum non-orthogonal angle (in degrees) at which second order discretisation is used. Above this angle first order discretisation is used.
'order'	Yes	•	'first' 'second' 'euler_second' 'central'	Sets the order of the spatial discretisation.
'central blend'	Yes	0.8	Float between 0.0 and 1.0	Coefficient of blending between first and second order terms.

Example usage:

```
parameters = {
  ..
  # Use the viscous equation set
  'equations' : 'viscous',
  'viscous' : {
    'relax' : 0.5,
    'correction' : 'over relaxed',
    'correction limiter' : 0.5,
    'gradient limiter type' : 'cell md',
    'gradient limiter' : 0.5,
    'max second order non orthogonal angle' : 70.0,
    'order' : 'second',
    'central blend' : 0.8,
    'first order cycles' : 100,
    'linear gradients' : False,
    'Inviscid Flux Scheme' : 'HLLC',
  },
}
```

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```

}

```

RANS

The fully turbulent (Reynolds Averaged Navier-Stokes Equations)

As well as the “*common*” settings, the ‘**RANS**’ equation set requires the additional ‘**turbulence**’ dictionary, which can have the following parameters:

Keyword	Required	Default	Valid values	Description
‘les’	Yes	‘none’	‘none’ ‘DES’ ‘DDES’ ‘IDDES’ ‘SAS’	Selects the hybrid RANS/LES model.
‘model’	Yes	–	‘sst’ ‘sas’ ‘sa-neg’ ‘sst-transition’	Selects the RANS turbulence model
‘approximate sa from sst results’	No		True False	Restart an SA-neg calculation from an SST solution
‘rotation correction’	No	False	True False	Adds the rotation correction term to SST or SA-neg
‘limit gradient k’	No		Float from 0.01 to 1	Activates the \bar{v} gradient limiter in the SA-neg model
‘qcr’	No	Off	2000 2020 2021	Activates the non-linear QCR correction to the turbulent stress. Applicable to both SST and SA-neg

les

Selects the hybrid RANS/LES model in the RANS solver which is applied to the base model selected with the “**model**” key word.

Setting	Notes
‘none’	Solve the RANS equations with no hybrid RANS/LES model
‘DES’	Detached Eddy Simulation
‘DDES’	Delayed Detached Eddy Simulation
‘IDDES’	Improved Delayed Detached Eddy Simulation
‘SAS’	Scale Adaptive Simulation

model

Selects the RANS turbulence model.

Setting	Notes
'sst'	The Menter Shear Stress Transport Turbulence Model (https://turbmodels.larc.nasa.gov/sst.html)
'sa'	Spalart-Allmaras turbulence model (https://turbmodels.larc.nasa.gov/spalart.html)
'sa-neg'	Negative Spalart-Allmaras turbulence model (https://turbmodels.larc.nasa.gov/spalart.html)
'sst-transition'	The Langtry-Menter 4-equation Transitional SST Model (https://turbmodels.larc.nasa.gov/langtrymenter_4eqn.html)

limit gradient k

Activates the $\tilde{\nu}$ gradient limiter in the SA-neg model. This helps eliminate gradient under/over shoot in regions of poor mesh quality.

The value should be between 0 and 1. **0** is off and **1** is maximum limiting.

qcr

Activates the non-linear QCR correction to the turbulent stress. Applicable to both SST and SA-neg. QCR has been shown to improve the prediction of separated corner flows, particularly on highly loaded wings. Three versions of the QCR model are available: [QCR 2000](#), [QCR 2020](#) and [QCR 2021](#).

Example RANS usage:

```
parameters = {
  ..
  # Use the viscous equation set
  'equations' : 'RANS',
  'RANS': {
    'order' : 'second',
    'first order cycles': 100,
    'freeze limiter cycle': 500,
    'linear gradients' : False,
    'leastq gradients' : False,
    'Inviscid Flux Scheme': 'HLLC',
    'roe low dissipation sensor': 'DES',
    'roe dissipation sensor minimum': 0.05,
    'turbulence' : {
      'model' : 'sst',
      # No Hybrid RANS/LES
      'les' : 'none',
      'rotation correction': False,
      'limit gradient k': 0.5
      'qcr': 2020
    },
  },
  ..
}
```

Advanced parameters for turbulence models

The following parameters can be used in the 'turbulence' dictionary to allow tuning of the turbulence models in zCFD. These are advanced parameters and shouldn't normally need to be adjusted.

Keyword	Required	Default	Valid values	Description
'betastar'	No	0.09	Positive number	Constant in the dissipation term on the k equation in the SST model
'cdes_kw'	No	0.78	Positive number	The $k-\omega$ part of the blended C_{DES} in SST
'cdes_keps'	No	0.21	Positive number	The $k-\epsilon$ part of the blended C_{DES} in SST
'cd1'	No	20	Positive number	Constant in the f_{dt} blending function in DDES and IDDES
'cd2'	No	3	Positive integer	Constant in the f_{dt} blending function in DDES and IDDES
'cw'	No	0.15	Positive number	Constant in the length scale calculation in IDDES
'a1'	No	0.31	Positive integer	Constant in the eddy viscosity limiter in SST
'production'	No	0	Positive integer	Selects the model for the production term in the SST model. See Production Term Table below
'rotation correction'	No	•	True False	Adds the rotation correction term to SST or SA-neg
'cdes'	No	0.65	Positive number	C_{DES} constant used for SA-neg based hybrid RANS/LES models
'ca1'	No	2.0	Positive number	Constant in the production of the gamma equation in the transition model in the compressible solver
'ca2'	No	0.06	Positive number	Constant in the destruction term for gamma equation in the transition model in the compressible solver
'ce1'	No	1.0	Positive number	Constant in the production of the epsilon equation in the transition model in the compressible solver
'ce2'	No	50.0	Positive number	Constant in the destruction term for gamma equation in the transition model in the compressible solver
'ctheta'	No	0.03	Positive number	Constant in the Re-theta transition correlation in the transition model in the compressible solver
'sigmagamma'	No	1.0	Positive number	Constant in the transition model in the compressible solver
'sigmatheta'	No	2.0	Positive number	Constant in the transition model in the compressible solver
'limit gradient k'	No	0.5	Positive number	Gradient limiter for the turbulent kinetic energy in the SA-neg model. A value of 0 turns off the limiter, 1 is maximum limiting
'separation correction'	No	True False	Boolean	Activates the separation correction for the transition model in the compressible solver
'qcr'	No	•	'2000'	Selects the QCR model for

'production' can have the following values:

Setting	Notes
0	Selects the vorticity based production term (SST-V) $P_m = \mu_t \Omega_v^2 - \frac{2}{3} \rho k \delta_{ij} \frac{\partial u_i}{\partial x_j}$
1	Selects the strain based production term for incompressible flows $P_m = \mu_t S^2$
2	Selects the strain based production term for compressible flows $P_m = \mu_t S^2 - \frac{2}{3} \rho k \delta_{ij} \frac{\partial u_i}{\partial x_j}$
3	Selects the Kato-Launder source term $P_m = \mu_t S \Omega_v - \frac{2}{3} \rho k \delta_{ij} \frac{\partial u_i}{\partial x_j}$

Incompressible RANS

Incompressible RANS equations follow the same structure as the compressible RANS equations with in addition to the parameters described in the *Incompressible Viscous* section. Note that the **scheme** block is not required, and that the turbulence model can have a different relaxation parameter to the main equation block.

Example incompressible RANS usage:

```
parameters = {
  ..
  # Use the incompressible RANS equation set
  'equations' : 'incomp RANS',
  'incomp RANS': {
    'relax' : 0.5,
    'correction' : 'over relaxed',
    'correction limiter' : 0.5,
    'gradient limiter type' : 'cell md',
    'gradient limiter' : 0.5,
    'max second order non orthogonal angle' : 70.0,
    'order' : 'second',
    'central blend' : 0.8,
    'first order cycles': 100,

    'turbulence' : {
      'model' : 'sst',
      'relax': 0.2,
    },
  },
  ..
}
```

LES

As well as the *“common”* settings, the **'LES'** equation set requires the additional **'turbulence'** dictionary, which can have the following parameters:

Keyword	Required	Default	Valid values	Description
'les'	Yes	'none'	'none' 'WALE'	Selects the hybrid RANS/LES model.

les

Selects the model for the subgrid eddy viscosity in the LES solver: either “**none**” for implicit LES or “**WALE**” to use the Wall Adapted Local Eddy Viscosity model.

Example usage:

```
parameters = {
  ..
  # Use the viscous equation set
  'equations' : 'LES',
  'LES': {
    'order' : 'second',
    'first order cycles': 100,
    'freeze limiter cycle': 500,
    'linear gradients' : False,
    'leastsq gradients' : False,
    'Inviscid Flux Scheme': 'HLLC',
    'roe low dissipation sensor': 'DES',
    'roe dissipation sensor minimum': 0.05,
    'turbulence' : {
      'les' : 'none',
    },
  },
  ...
}
```

Incompressible LES

Incompressible LES equations follow the same structure as the compressible LES equations with the addition of the parameters described in the *Incompressible Viscous* section. Note that the scheme block is not required, and that the turbulence model can have a different relaxation parameter to the main equation block.

Example incompressible LES usage:

```
parameters = {
  ..
  # Use the incompressible LES equation set
  'equations' : 'incomp LES',
  'incomp LES': {
    'relax' : 0.7,
    'order' : 'second',
    'first order cycles': 100,
    'turbulence' : {
      'les' : 'DES',
      'relax' : 0.2,
    },
  },
  ...
}
```

1.5.6 Fluid-structure interaction

zCFD has the capability of simulating Fluid Structure Interaction (FSI) using both a modal model, as well as any generic full FEA program through the use of our generic coupling scheme.

Keyword	Re-quire	Default	Valid values	Description
'type'	Yes		'generic'	FSI driver to be used when coupling to an FEA code
'zone'	Yes		List of zone ID integers	Which boundaries within the aerodynamic mesh are moving structural boundaries
'fixed zones'	Yes		List of zone ID integers	Which boundaries should not be moved by any mesh deformation
'transform type'	Yes		'rbf multiscale' 'rbf' 'IDW'	Interpolation method to be used.
'alpha'	Yes	1	Float	Support radius used by RBF
'basis'	Yes	'c2'	'c2' 'c4' 'c0' 'tps' 'gaussian'	Which basis function to use for RBF
'base point fraction'	Yes	0.1	Float	Number of points to use in the reduced base set for rbf multiscale interpolation
'tol'	Yes	0.01	Float	Set the target error tolerance for the rbf interpolation
'max error'	Yes	0.1	Float	Set the maximum initial error tolerance for rbf interpolation
'n nearest'	Yes	100	Positive integer	Number of points to be used in IDW interpolation
'deformation distance'	Yes	1	Float	Set the maximum support radius for IDW interpolation
'blending stiffness'	Yes	0.5	Float	Set the blending stiffness for the IDW interpolation
'power'	Yes	[3.0,5.0,10.0]	Set the IDW power for the nearfield and farfield boundaries, and the power between them.	List of Float
'user variables'	No	{}	Dict of variables to values	Custom parameters passed into the generic FSI code

type

Specifies which FSI driver should be used when coupling to an FEA code, **'generic'**. This tells zCFD which FSI python file should be used to execute the FSI coupling: **'generic'** will use the **genericFSI.py** interface that should be implemented to meet your requirements. Out the box **genericFSI.py** will not perform any changes.

zone

zone should be a list of zone IDs, these specify which surface is the moving FSI surface. This provides methods to extract surface normals, pressure forces, and cell centres from the specified cells, as well as allowing these surface points to drive mesh deformations in the volume mesh.

For RBF, this must include any static zones, where the motion of a static zone is set to 0.

fixed zones

fixed zones should be a list of zone IDs, these specify surfaces which must remain fixed, such as an interface, periodic boundary, or symmetry plane, these surfaces will remain untouched by the IDW mesh motion interpolation.

Note

IDW only

transform type

In FSI simulations the active surface defined in the 'zone' block, will move relative to the rest of the mesh. In order to maintain a conformal volume mesh, these displacements must be interpolated into the volume mesh. **transform type** defines which interpolation scheme should be used.

Setting	Notes
'rbf'	Radial Basis Functions require the solving of a linear system, where a continuous function is fitted between all points which defines the motion. This function can then be evaluated at other points within the domain to get the interpolated values.
'rbf multiscale'	RBF multiscale uses the a multiscale algorithm using a varying support radius to reduce the number of nodes in the linear system, where as RBF uses a Greedy algorithm.
'IDW'	Inverse Distance Weighting does not require the solving of a linear system, and instead represents a function using a weighted sum of nearby function values.

Note

'rbf multiscale' has generally superseded the greedy algorithm, used in 'rbf', in terms of both speed performance and accuracy, so is the preferred RBF option.

alpha

Only applies to 'rbf' and 'rbf multiscale' interpolation schemes.

'alpha' sets the support radius used by the RBF. The Radial Basis Function used in RBF interpolation will have a set support radius defining the 1D shape of the function as a function of r. This determines the region of influence for the function. Compact functions such as C0, C2, C4 have a maximum radius, outside of which the influence of the RBF is 0. For functions with global influence such as Gaussian and TPS, alpha becomes the normalisation factor - i.e. when $r = \alpha$, $e = 1$ if $rbf = f(e)$.

'alpha' should be larger than the maximum anticipated deformation.

basis

Only applies to 'rbf' and 'rbf multiscale' interpolation schemes.

When performing RBF interpolation a specific function needs to be defined to create the interpolant. Compact functions such as C0, C2, C4 have a maximum region of influence, Gaussian and TPS have global influence.

Note

For 99% of applications C2 works best

base point fraction

Only applies to 'rbf' and 'rbf multiscale' interpolation schemes.

Solving the RBF system requires solving an NxN sized linear system, where N is the number of moving nodes- i.e. nodes on the surface [4] defined earlier. For large meshes this quickly becomes prohibitively expensive,

therefor it is desirable to solve a reduced set of points. The Multiscale method is a ‘reduced base set method’ where the linear system is only solved on the base set of nodes, with the remaining nodes solved iteratively. ‘**base point fraction**’ dictates how many nodes of the full set should be included in the base set. Setting the base point fraction to 1.0 returns a standard full RBF.

tol

Only applies to ‘**rbf**’ interpolation scheme.

At each point selection step during Greedy selection, the interpolation problem is solved on the current base set of data. From this the error between the exact solution and interpolated solution for all points in the mesh is identified, this value is used as the initial guess for the ‘worst’ error within the mesh. Once the total error is below this tolerance, the greedy point selection is complete.

max error

Only applies to ‘**rbf**’ interpolation scheme.

At each point selection step during Greedy selection, the interpolation problem is solved on the current base set of data. From this the error between the exact solution and interpolated solution for all points in the mesh is identified. If this error is greater than the max error specified here, an error message is thrown.

n nearest

Only applies to ‘**IDW**’ interpolation scheme.

When using IDW mapping, the deformation of each surface point is mapped onto a set number of volume points, with the value determined by the weighted inverse distance between the donor and the recipient.

deformation distance

Only applies to ‘**IDW**’ interpolation scheme.

Sets the maximum region of influence for the inverse distance weighting mapping. If there are fewer than “n” neighbours within a distance “d”, then only neighbours within that distance are used.

blending stiffness

Only applies to ‘**IDW**’ interpolation scheme.

Set the blending stiffness for the IDW interpolation.

power

Only applies to ‘**IDW**’ interpolation scheme.

Set the IDW power for the nearfield and farfield boundaries, and the power between them.

user variables

If you had additional variables for time marching scheme or FSI control (e.g. file names) you may want to pass as variables to the **genericFSI.py** script, these should be included in this dictionary.

1.5.7 Material Specification

This dictionary sets the material properties of the fluid being modelled. The default values are those of air, but the dictionary can be modified to model any ideal, compressible, perfect gas.

Keyword	Re-quired	Default	Valid values
'sutherlands const'	Yes	110.4	Float
'prandtl no'	Yes	0.72	Float
'gas constant'	Yes	287	Float
'gamma'	Yes	1.4	Float
'turbulent prandtl no'	Yes	0.9	Float
'gravity'	No		Vector

Example usage:

```
parameters = {
..
'material' : 'air',
'air' : {
    'gamma' : 1.4,
    'gas constant' : 287.0,
    'Sutherlands const': 110.4,
    'Prandtl No' : 0.72,
    'Turbulent Prandtl No' : 0.9,
},
..
}
```

sutherlands const

This option controls the variation of the viscosity of the fluid with temperature.

Sutherland's law: $\mu = \mu_{ref} \left(\frac{T}{T_{ref}} \right)^{3/2} \frac{T_{ref} + S}{T + S}$, where S is Sutherland's constant.

In zCFD, T_{ref} and μ_{ref} are given by the *reference* initial condition dictionary, where T is specified directly and μ is specified either directly via **'viscosity'** or indirectly via **'reynolds no'**.

Typically for air $\mu_{ref} = 1.716e - 5$ and $T_{ref} = 273.15$

For more information: https://www.cfd-online.com/Wiki/Sutherland%27s_law

prandtl no

This option sets the Prandtl number, a non-dimensional number which is the ratio of momentum and thermal diffusivities in a fluid. In zCFD, where μ and c_p are already set, setting the Prandtl number has the effect of setting the thermal conductivity, k , of the fluid.

$$\text{Pr} = \frac{\text{momentum diffusivity}}{\text{thermal diffusivity}} = \frac{c_p \mu}{k}$$

This can also be considered as $\text{Pr} = \frac{\text{Thickness of thermal boundary layer}}{\text{Thickness of fluid boundary layer}}$

gas constant

This changes R , the gas constant of the fluid. Different fluids have different molecular masses, and therefore different gas constants. 287.1 is appropriate for air.

Constant pressure and constant volume specific heats, c_p and c_v , are set by *gamma* and R according to the following relationships:

$$c_p = \frac{\gamma - 1}{\gamma} R$$

$$\gamma = \frac{c_p}{c_v}$$

gamma

This changes γ , the ratio of specific heats of the fluid. 1.4 is appropriate for air, but a value of 1.33 is often used for combustion exhaust gases.

turbulent prandtl no

This changes the turbulent Prandtl number of the fluid being modelled.

In simulations which model turbulence viscosity (RANS, LES and other scale resolving simulations), the eddy viscosity, μ_t accounts for the additional diffusivity of momentum due to turbulence relative to the equivalent laminar flow. There is likewise additional diffusivity of heat due to turbulence relative to the equivalent laminar flow, and the turbulent prandtl number accounts for this.

In an eddy viscosity based simulation, $Pr_t = \frac{c_p \mu_t}{k_t}$

gravity

This sets the direction in which gravity acts in your simulation. For most industrial and aerospace flows, buoyancy effects are not important and therefore buoyancy should not be set. However, certain flows (e.g. plumes) do require buoyancy effects for accurate modelling.

gravity is specified as x,y,z vector, for example “[0,0,-9.81]”

1.5.8 Initial Conditions

An initial condition dictionary defines a fluid state. They are used to provide a reference initial state for the solution as well as specific conditions that can be assigned to *boundary conditions*.

Initial condition properties are defined using consecutively numbered blocks

```
'IC_1' : { ... },
'IC_2' : { ... },
```

By default zCFD will use the “IC_1” block to provide initial flow field conditions for the simulation but this can be changed with the *initial* parameter.

In addition to fully describing a set of conditions, zCFD allows you to specify *reference conditions* to be specified relative to a base set. This is typically used to set conditions for flow entering (inflow) or leaving (outflow) the domain.

Another way of prescribing an initial condition is by defining a dynamic *driving function*, which on evaluation returns an initial condition dictionary.

Keyword	Re-quired	Default	Valid values	Description
'pressure'	Yes		Float	Static pressure in Pascals. Used to compute density and set Total Energy in the Compressible solver.
'temperature'	Yes		Float	Static temperature in Kelvin. Used to compute density and for dynamic viscosity scaling using Sutherlands law.
'V'	Yes		Dict	See Velocity
'reynolds no'	When 'viscosity' not set.		Float	Used to calculate viscosity at supplied temperature
'reference length'	No	1	Float	Reference length to be used to calculate viscosity from the Reynolds number
'viscosity'	When 'reynolds no' not set.		Float	Sets the dynamic viscosity at the temperature with scaling provided by Sutherlands law defined in material section.
<i>'turbulence intensity'</i>	No		Float	Turbulence intensity (%)
<i>'eddy viscosity ratio'</i>	No	0.01	Float	Ratio of dynamic viscosity to turbulent viscosity used to set the turbulence quantities
<i>'ambient turbulence intensity'</i>	No	0.1	Float	Value of background turbulence intensity (%) to maintain in fluid
<i>'ambient eddy viscosity ratio'</i>	No	1e-20	Float	Value of background turbulence eddy viscosity ratio to maintain in fluid
'profile'	No	1e-20	Dict	See Velocity Profile

Example usage:

```
parameters = {
..
"IC_1": {
  "V": {"vector": [0.0, 2.5, 0.0] },
  "ambient eddy viscosity ratio": 1e-20,
  "ambient turbulence intensity": 1e-20,
  "eddy viscosity ratio": 0.1,
  "pressure": 101325.0,
  "temperature": 273.15,
  "turbulence intensity": 0.01,
  "viscosity": 1.79e-05,
..
},
```

Velocity

Velocity can be specified in two ways, either a vector or a vector and a Mach number. When Mach number is specified the velocity direction is provided by the vector and the velocity magnitude is computed from the Mach number and speed of sound at the pressure and temperature provided.

For example to set a velocity of 50 mesh units/sec in the X direction:

```
..
"V" : {"vector": [50.0,0.0,0.0]}
..
```

Or to set a velocity of mach 0.2 in the X direction:

```
..
"V" : {"vector": [1.0,0.0,0.0], "mach": 0.2}
..
```

Viscosity

Dynamic (shear, absolute or molecular) viscosity should be defined at the static temperature previously specified. This can be specified either as a dimensional quantity or by a Reynolds number and reference length

```
# Dynamic viscosity in dimensional units
'velocity' : 1.83e-5,
```

or

```
# Reynolds number
'reynolds No' : 5.0e6,
# Reference length
'reference length' : 1.0,
```

Note

Reynolds number is defined as: $Re = \frac{\text{density} * V * \text{referencelength}}{\text{viscosity}}$

Turbulence intensity & Eddy viscosity

Turbulence intensity is defined as the ratio of velocity fluctuations u' to the mean flow velocity. A turbulence intensity of 1% is considered low and greater than 10% is considered high.

```
# Turbulence intensity %
'turbulence intensity': 0.01,
# Turbulence intensity for sustainment %
'ambient turbulence intensity': 0.01,
```

The eddy viscosity ratio (μ_t/μ) varies depending type of flow. For external flows this ratio varies from 0.1 to 1 (wind tunnel 1 to 10)

For internal flows there is greater dependence on Reynolds number as the largest eddies in the flow are limited by the characteristic lengths of the geometry (e.g. The height of the channel or diameter of the pipe). Typical values are:

Re	3000	5000	10,000	15,000	20,000	> 100,000
eddy	11.6	16.5	26.7	34.0	50.1	100

```
# Eddy viscosity ratio
'eddy viscosity ratio': 0.1,
# Eddy viscosity ratio for sustainment
'ambient eddy viscosity ratio': 0.1,
```

Velocity Profile

The user can also provide functions to specify a 'wall-function' - or the turbulence viscosity profile near a boundary.

Keyword	Re-quired	Default	Valid values	Description
'abl'	No		Dict	Specify an <i>ABL</i> (Atmospheric Boundary Layer)
<i>'field'</i>	No		File name	Specify a field of data that is used as a lookup for setting the flow conditions.
'use wall distance'	No	False	True/False	Use wall distance in place of z coordinate in field during interpolation process. This can be used in setting the profile of flows on a terrain mesh with a variable ground location at the boundary

field

The file specified using the 'field' parameter should be in the ParaView/VTK VTP format. It should contain a node array with one or more of the following array names: 'Pressure', 'Temperature', 'Velocity', 'TI' and 'EddyViscosity'. zCFD will then look up those values in the solution by looking up the nearest point in the VTP file.

```
..
'profile' : {
  'field' : 'inflow_field.vtp',
  # Localise field using wall distance rather than z coordinate
  'use wall distance' : True,
},
..
```

Note

Note the field will override the conditions specified previously therefore the user can specify only the conditions that are different from default.

ABL

Keyword	Re-quired	Default	Valid values	Description
'roughness length'	No		Float	It is a measure of the height at which the mean velocity of the wind becomes zero, due to the frictional effects between the air and the surface.
'friction velocity'	No		Float	Specify the friction velocity at the surface.
'surface layer height'	No		Float	The surface layer height, also known as the aerodynamic or boundary layer height.
'monin-obukhov length'	No		Float	The Monin-Obukhov length.
'tke'	No		Float	Set the turbulent kinetic energy.
'z0'	No		Float	Set the z location of the ground rather than using the z coordinate in the mesh.
'up'	No	[0,0,1]	Vector	Direction of gravity

roughness length

Is a measure of the height at which the mean velocity of the wind becomes zero, due to the frictional effects between the air and the surface.

The roughness length is typically denoted by the symbol " z_o " and is defined as the vertical distance between the Earth's surface and the height at which the logarithmic wind profile intersects the surface. The logarithmic wind profile is a mathematical relationship that describes the variation of wind speed with height in the atmospheric boundary layer.

The roughness length depends on the surface characteristics of the terrain or objects present on the Earth's surface. Different surfaces, such as forests, urban areas, or bodies of water, have different roughness lengths. For example, a smooth surface like open water would have a small roughness length, while a densely forested area would have a larger roughness length.

The wall boundary mesh is assumed to be at the height of the roughness length rather than ground level and therefore the first cell height should not be smaller than the roughness length.

friction velocity

Friction velocity, often denoted as " u_\star " (pronounced "u-star"), is another important parameter in the study of atmospheric boundary layers. It represents the characteristic velocity of turbulent motions in the surface layer of the atmosphere, generated by the shear stress between the air and the Earth's surface.

Friction velocity is defined as the square root of the shear stress divided by the air density:

$$u_\star = \sqrt{\frac{\tau}{\rho}}$$

where:

- u_\star is the friction velocity,
- τ is the shear stress between the air and the surface, and

- ρ is the density of the air.

The shear stress, τ , arises from the momentum transfer between the moving air and the surface roughness elements. It is related to the wind speed and the roughness length through a logarithmic wind profile, described by the following equation:

$$u(z) = \left(\frac{u^*}{\kappa}\right) * \ln \frac{z}{z_o}$$

where:

- $u(z)$ is the wind speed at height z above the surface,
- κ is the von Kármán constant (approximately 0.4), and
- z_o is the roughness length.

The friction velocity provides a measure of the intensity of turbulence near the Earth's surface. It influences several atmospheric processes, including heat and moisture exchange, pollutant dispersion, and the formation of atmospheric boundary layer structures. The magnitude of the friction velocity depends on surface roughness, wind speed, and atmospheric stability, among other factors.

surface layer height

The surface layer height, also known as the aerodynamic or boundary layer height, refers to the vertical extent of the atmospheric boundary layer near the Earth's surface. It represents the region where the physical properties, such as wind speed, temperature, humidity, and turbulence, are influenced by the underlying surface. The height of the surface layer is often estimated based on empirical relationships or atmospheric stability conditions. It can vary from a few meters to a few hundred meters above the ground, depending on factors such as surface roughness length, wind speed, and atmospheric stability. Additionally, the surface layer height can change diurnally, with variations due to daytime heating and nighttime cooling effects.

monin-obukhov length

The Monin-Obukhov length, often denoted as “ L ”, is a parameter used in the study of atmospheric boundary layers to characterise the stability of the air near the Earth's surface. It is named after the Russian scientists A. S. Monin and A. M. Obukhov, who made significant contributions to the understanding of turbulence and boundary layer physics.

The Monin-Obukhov length is defined as the ratio of the potential temperature difference to the buoyancy flux. It is given by the following equation:

$$L = -\frac{u^*{}^3 * \theta_v}{\kappa * g * w\theta}$$

where:

- L is the Monin-Obukhov length,
- u^* is the friction velocity,
- θ_v is the virtual potential temperature,
- κ is the von Kármán constant (approximately 0.4),
- g is the acceleration due to gravity, and
- $w\theta$ is the vertical flux of virtual potential temperature.

The Monin-Obukhov length is an indicator of atmospheric stability. It quantifies the relationship between the mechanical production of turbulence due to wind shear and the buoyancy effects caused by vertical temperature gradients. Positive values of L indicate stable atmospheric conditions, while negative values indicate unstable conditions. A neutral atmosphere corresponds to $L = 0$.

The Monin-Obukhov length influences various atmospheric processes, such as turbulence structure, heat and moisture exchange, and dispersion of pollutants. It plays a significant role in determining the behaviour of the atmospheric boundary layer, including the vertical mixing of air masses and the development of turbulence. The value of L is influenced by factors such as surface properties, wind speed, temperature, and humidity gradients.

1.5.9 Reference Conditions

Reference Conditions enable a set of conditions to be specified relative to a base set of *initial conditions*. This is typically used to set conditions for flow entering (inflow) or leaving (outflow) the domain

Reference condition properties are defined in the same way as initial conditions using consecutively numbered blocks.

```
'IC_2' : {...},
'IC_3' : {...},
```

Note

Reference conditions can not be used for “IC_1”

Keyword	Re-quired	Default	Valid values	Description
'reference'	Yes		Float	Specify the base condition as the reference for this set of conditions
'static pressure ratio'	No		Float or <i>Function</i> or <i>File</i>	Set the static pressure using a ratio relative to the reference static pressure. Where static pressure = reference static pressure * static pressure ratio
'total pressure ratio'	No		Float or <i>Function</i> or <i>File</i>	Set the total pressure using a ratio relative to the reference total pressure. Where total pressure = reference total pressure * total pressure ratio
'total temperature ratio'	No		Float or <i>Function</i> or <i>File</i>	Set the total temperature using a ratio relative to the reference total temperature. Where total temperature = reference total temperature * total temperature ratio
'mass flow ratio'	No		Float	Specify a <i>mass flow</i> ratio.
'mass flow rate'	No		Float	Specify a <i>mass flow</i> rate.
'vector'	No		[X, Y, Z] or <i>Function</i>	Specify direction vector used to specify the direction of the flow for specific boundary conditions.
'mach'	No		Float	Specify a mach number used for specific boundary conditions like inflows/jets.

Example usage:

```
parameters = {
..
'IC_2' : {
    'reference' : 'IC_1',
    'total temperature ratio' : 1.0,
    'mass flow rate' : 10.0,
    'vector' : [1,0,0],
```

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```
'mach' : 0.5,
},
..
},
```

Mass Flow

Mass flow ratio is defined as:

$$ratio = (density * area * V) / (density_{ref} * area * V_{ref}) = (density * V) / (density_{ref} * V_{ref})$$

Mass flow rate is defined as:

$$\dot{m} = density * area * V$$

Note

Note area is in mesh units squared

Using a file

A file can be used to provide a lookup for the pressure and temperature ratios. This file should be in the Paraview/VTK VTP format. The file should contain a surface with specific values as node arrays data. zCFD then looks up the values by finding the nearest point to the mesh location.

The node array data in the VTP should be named specifically for each keyword:

Keyword	Node Array Name
'static pressure ratio'	StaticPressureRatio
'total pressure ratio'	TotalPressureRatio
'total temperature ratio'	TotalTemperatureRatio

1.5.10 Fluid Zones

The fluidic zone properties are defined using consecutively numbered blocks like:

```
'FZ_1' : {...},
'FZ_2' : {...},
'FZ_3' : {...},
```

Each block corresponds to a specific fluid zone within the simulation domain and is identified by a unique key (e.g., 'FZ_1'). The properties within each block specify the type of zone (such as translating, rotating, porous, disc, or canopy) and the relevant parameters required for that zone type. These parameters control the physical behaviour and characteristics of the fluid zone, such as velocity vectors, resistance factors, geometric definitions, and other model-specific settings.

The configuration allows for flexible definition of multiple fluid zones, each with its own set of properties, to accurately represent complex flow regions within the computational mesh.

For translating regions

```
'FZ_1':{
  'type':'translating',
  # Use def when the vtp file specifies a closed volumetric region defining the
  -translating region
  'def':'translating.vtp',
  # Use zone when the mesh containns a predefined cell zone
```

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```

'zone': [10],
# Velocity vector in mesh units/sec
'vector': [1.0, 0.0, 0.0],
},

```

For rotating regions

```

'FZ_1':{
  'type':'rotating',
  # Use def when the vtp file specifies a closed volumetric region defining the
  -rotating region
  'def':'rotating.vtp',
  # Use zone when the mesh containns a predefined cell zone
  'zone': [10],
  'omega': -0.52, # rad/s
  'axis': [1.0, 0.0, 0.0],
  'origin': [0.0, 0.0, 0.0],
},

```

For porous regions

```

'FZ_1':{
  'type':'porous',
  # Use def when the vtp file specifies a closed volumetric region defining the
  -porous region
  'def':'porous.vtp',
  # Use zone when the mesh containns a predefined cell zone
  'zone': [10],
  # Inertial resistance factor
  'C2': 500,
  # Permeability
  'alpha': 10e-7,
},

```

Note

The model constants need to be provided in mesh units. The examples below assume a mesh in metres (Units of alpha is $1/m'$ and C_2 is $1/m^2'$)

The momentum source term for porous media is given by:

$$S_i = -\left(\frac{\mu}{\alpha} V_i + \frac{1}{2} \rho C_2 |V| V_i\right)$$

where S_i is the source term in the i -th direction, μ is the dynamic viscosity, α is the permeability, ρ is the fluid density, C_2 is the inertial resistance factor, and V_i is the velocity component.

In laminar flow using Darcy's power law:

$$\Delta P = \frac{\mu}{\alpha} V$$

where ΔP is the pressure drop, μ is the dynamic viscosity, α is the permeability, and V is the velocity.

Table 1.2: Example Permeability Values

Material	Permeability α (m^2)
Fence	1×10^{-7}
Car radiator	1×10^{-9}
Sand	1×10^{-11}

Table 1.3: Example Inertial Resistance Factor (C2) Values

Material	C2 (1/m)
Open cell foam	1000
Gravel	500
Sand	100
Fine mesh	10000

For actuator disk zones

Note

The actuator disk model is a simplified representation of a rotating disc that generates thrust and drag forces in a fluid flow. It is commonly used in computational fluid dynamics (CFD) simulations to model the effects of wind turbines, propellers, or other rotating machinery on the surrounding fluid.

The simple actuator disk model assumes that the disc has a uniform distribution of thrust and drag forces across its surface. The thrust coefficient (CT) and tip speed ratio (TSR) are key parameters that define the performance of the actuator disk. The thrust coefficient (CT) is a dimensionless parameter that relates the thrust force generated by the disc to the dynamic pressure of the incoming flow. It is defined as:

$$CT = \frac{T}{\frac{1}{2}\rho V^2 A}$$

where T is the thrust force, ρ is the fluid density, V is the velocity of the incoming flow, and A is the area of the disc.

```
'FZ_1':{
  'type':'disc',
  "discretisation": {"type": "disc", "number of elements": 24},
  "model": {
    # simple or BET
    "type": "simple",
    # Thrust coefficient
    'thrust coefficient':0.84,
    # Power coefficient
    'power coefficient':0.84,
  },
  "controller": {
    # none, tsr curve, fixed, schedule
    "type": "none",
  },
  "geometry": {
    # Thrust direction
    "normal": [0.0, 0.0, 1.0],
    # Disc centre
    "centre": [0.0, 0.0, 1e-06],
    # Up vector
    "up": [1.0, 0.0, 0.0],
    # Inner radius
    "inner radius": 0.039025,
    # Outer radius
    "outer radius": 0.175,
  },
  "name": "R01",
}
```

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```

# Rotation direction clockwise or anticlockwise
"rotation direction": "clockwise",
# closed surface defining region of cells to distribute momentum source
'def': 'T38-248.75.vtp',
# Location of reference conditions used to calculate thrust from disc
'reference point': [1.0,1.0,1.0],
# Rotational speed
'omega': 314.1592653589793, # rad/s
},

```

Blade Element Theory (BET) actuator disk model The BET actuator disk model is a more advanced representation of a rotating disc that takes into account the aerodynamic characteristics of the blades or elements on the disc. It is commonly used in simulations of wind turbines, propellers, and other rotating machinery to accurately predict their performance in fluid flows. The BET model divides the disc into multiple sections or elements, each with its own aerodynamic properties. The thrust and drag forces are calculated for each element based on its local angle of attack, lift and drag coefficients, and other parameters. This allows for a more detailed representation of the flow around the disc and the interaction between the blades and the fluid.

```

"FZ_1": {
  "type": "disc",
  "discretisation": {"type": "disc", "number of elements": 24},
  "model": {
    # simple or BET
    "type": "BET",
    # propellor or turbine
    "kind": "propellor",
    # Blade chord (span %, chord length)
    "blade chord": [
      [0.2333, 0.1468],
      [0.2667, 0.1681],
      [0.3333, 0.211],
      [0.4, 0.2261],
      [0.4667, 0.2271],
      [0.5333, 0.2208],
      [0.6, 0.2091],
      [0.6667, 0.1926],
      [0.7333, 0.1715],
      [0.8, 0.1462],
      [0.8667, 0.1212],
      [0.9091, 0.1027],
      [1.0, 0.0581],
    ],
    # Blade twist (span %, angle degrees)
    "blade twist": [
      [0.2333, 28.6202],
      [0.2667, 25.5228],
      [0.3333, 20.9055],
      [0.4, 18.3605],
      [0.4667, 16.665],
      [0.5333, 14.8896],
      [0.6, 13.4845],
      [0.6667, 12.3585],
      [0.7333, 11.4509],
      [0.8, 10.2263],
      [0.8667, 9.0608],
      [0.9091, 8.5419],
    ]
  }
}

```

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```

    [1.0, 0.0],
  ],
  # Number of circumferential sections
  "number of sections": 24,
  # Number of blades
  "number of blades": 2,
  # list of aerofoil sections [[spanwise %, airofoil_name1], ...] names should
  -correlate to entries in "aerofoils"
  "aerofoil positions": [[0.0, "aerofoil1"], [1.0, "aerofoil1"]],
  # Aerofoil data
  "aerofoils": {
    # dictionary of aerofoil coefficient tables
    "aerofoil1": {
      # drag polar in [degrees, cd]
      "cd": [
        [-60.0, 1.4552],
        [-50.0, 1.0992],
        [-40.0, 0.748],
        [-30.0, 0.4605],
        [-25.0, 0.3701],
        [-20.0, 0.284],
        [-15.0, 0.1842],
        [-10.0, 0.1157],
        [-6.0, 0.0883],
        [-5.0, 0.0806],
        [-4.0, 0.074],
        [-3.0, 0.0583],
        [-2.0, 0.0353],
        [-1.0, 0.0314],
        [0.0, 0.0289],
        [1.0, 0.0276],
        [2.0, 0.0291],
        [3.0, 0.0308],
        [4.0, 0.0333],
        [5.0, 0.0357],
        [6.0, 0.0409],
        [10.0, 0.0667],
        [15.0, 0.2908],
        [20.0, 0.4857],
        [25.0, 0.6023],
        [30.0, 0.7409],
        [40.0, 1.1456],
        [50.0, 1.8184],
        [60.0, 2.3542],
      ],
    },
  ],
  # lift polar in [degrees, cl]
  "cl": [
    [-60.0, -0.7978],
    [-50.0, -0.8195],
    [-40.0, -0.7204],
    [-30.0, -0.5429],
    [-25.0, -0.4336],
    [-20.0, -0.3499],
    [-15.0, -0.1601],
    [-10.0, -0.0623],
    [-6.0, -0.1109],
  ],

```

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```

        [-5.0, -0.1771],
        [-4.0, -0.146],
        [-3.0, -0.0018],
        [-2.0, 0.4084],
        [-1.0, 0.556],
        [0.0, 0.7093],
        [1.0, 0.8542],
        [2.0, 0.9736],
        [3.0, 1.0824],
        [4.0, 1.1568],
        [5.0, 1.2398],
        [6.0, 1.2964],
        [10.0, 1.5453],
        [15.0, 1.4509],
        [20.0, 1.5137],
        [25.0, 1.3547],
        [30.0, 1.3587],
        [40.0, 1.4378],
        [50.0, 1.5453],
        [60.0, 1.3818],
    ],
},
},
# Tip loss correction radius (span %)
"tip loss correction radius": 0.8,
# elliptic, acos-fit, accos shift-fit, f-fit, none, rstar
"tip loss correction": "rstar",
},
"controller": {
    # none, tsr curve, fixed, schedule
    "type": "fixed",
    # angular velocity
    "omega": 314.1592653589793,
    # blade pitch angle
    "pitch": 0.0
},
# Rotation direction clockwise or anticlockwise
"rotation direction": "clockwise",
# Geometry of the actuator disk
"geometry": {
    # Thrust direction
    "normal": [0.0, 0.0, 1.0],
    # Disc centre
    "centre": [0.0, 0.0, 1e-06],
    # Up vector
    "up": [1.0, 0.0, 0.0],
    # Inner radius
    "inner radius": 0.039025,
    # Outer radius
    "outer radius": 0.175,
},
"name": "R01",
"reference plane": True,
# "reference point": [0.0, 0.0, 0.0],
"status": "on",
"verbose": True,

```

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```

"update frequency": 1,
"output": True,
"def": "R01.vtp",
},

```

For tree canopies in terrain wind models

```

'FZ_1':{
    'type':'canopy',
    # Use def when the vtp file specifies a closed volumetric region defining the
    -canopy
    'def':'canopy_dacosta.vtp',
    # Use field when the vtp specifies a set of points on the surface (see below
    -for details)
    'field':'canopy_field.vtp',
    'func':lad_function,
    'cd':0.25,
    'beta_p':0.17,
    'beta_d':3.37,
    'Ceps_4':0.9,
    'Ceps_5':0.9,
},

```

where the parameters `cd`, `beta_p`, `beta_d`, `Ceps_4` and `Ceps_5` are defined in the literature (for example Desmond, 2014) and the leaf area density (LAD) is typically specified using a function

```

def lad_function(cell_centre_list):
    lai = 5.0 # for example following Da Costa 2007
    h_can = 20.0
    lad_list = []
    for cell in cell_centre_list:
        wall_distance = cell[3]
        lad = (np.interp(wall_distance, a_z[0] * h_can, a_z[1]) * lai / h_can,)
        lad_list.append(lad)

    return lad_list

```

and the variation in leaf area density is a function of height

```

a_z = (
    np.asarray([0.0,0.43,0.1,0.45,0.2,0.56,0.3,0.74,0.4,1.10,
                0.5,1.35,0.6,1.48,0.7,1.47,0.8,1.35,0.9,1.01,1.0,0.00]).reshape(11,
    -2).T
)

```

Note

When using the field specification the height of the canopy at each boundary face is set by finding the nearest point to the face centre on the supplied VTK file with the height value looked up in a node based scalar array called 'Height'

1.5.11 Mesh Transformation

This dictionary is used to setup an initial deformation of the mesh. Typically a known deformation of a surface in the mesh is propagated out into the volume using either radial basis function or inverse distance weighted interpolation. Deforming an aircraft wing or wind turbine blade to a static load shape are two uses of this functionality.

Keyword	Re-quire	Default	Valid values	Description
'type'	Yes		'rbf' 'rbf multiscale' 'idw'	Selects the <i>interpolation</i> method used.
'base point fraction'	No		Float	Fraction of points included in the base set when using ' rbf multiscale '
'alpha'	No		Float	Sets the support radius (the radius of influence) of the rbf surface points.
'zone'	Yes		List of zone ID integers	Sets a list of surface zones to deform
'fixed zones'	No		List of zone ID integers	Sets the surface zones which remain fixed in position when using ' idw ', useful if you have surfaces that are within the influence of the interpolation that should remain fixed.
'func'	Yes		<i>Transform Function</i>	A python function that describes the surface deformation to be propagated into the volume mesh. The function is called for each node on the surfaces specified in the 'zones' key.
'basis'	No		<i>c0</i> <i>c2</i> <i>tps</i> <i>gaussian</i>	Selects the type of radial basis function used. Can be Welland's <i>c0</i> or <i>c2</i> function, thin plate spline (<i>tps</i>) or Gaussian.
'tol'	No		Float	The maximum permissible distance error between the deformed surface shape and that obtained using the greedy ' rbf ' method. No more points will be added to the system once this tolerance is reached.
'power'	No	[3,5,10]	List of int	A list of three exponents used in the ' idw ' interpolation scheme.
'n nearest'	No	100	Int	The number of nodes closest to the current point used to determine the ' idw ' interpolation weight.
'deformation distance'	No	1	Float	The distance over which the surface deformation is blended into the volume mesh.
'blending stiffness'	No	0.5	Float	The stiffness of the blending function used to propagate the ' idw ' interpolation of the surface deformation into the volume mesh.

Interpolation method

Selects the interpolation method used to propagate the surface deformation into the volume mesh. Three methods are available:

'rbf' uses the 'greedy' method of [Allan et al.](#) where the deformation is started with a subset of points and additional points are added until the surface deformation reaches the requested tolerance.

'rbf multiscale' uses the [multiscale](#) rbf method where a subset of surface points with a fixed support radius are solved implicitly and the remaining points are solved explicitly with a support radius determined as part of the solution process. The fraction of points included in the base set can be set with **'base point fraction'**. The base set of points are assigned the support radius **'alpha'** and hence can have a wider sphere of influence than the remaining points which are used in the multiscale process.

Note

Increasing the number of points in the base set and/or increasing alpha generally makes the surface deformation propagate further into the volume mesh reducing the likelihood of generating poor quality cells

'idw' uses a simple inverse distance weighted interpolation. The **'power'** parameter can provide a list of three exponents used in the IDW scheme. The first (p1) is applied to the interpolation weight of points close to the surface, the second (p2) to points which are the deformation distance away from the surface and the third (p3) is used to blend between the two extremes.

$$wt_1 = (deformationdistance/distance)^{p1} \quad wt_2 = (deformationdistance/distance)^{p2} \quad blend = ((deformationdistance - distance)/deformationdistance)^{p3}$$

Then the weight is:

$$wt = (wt_1 * (1.0 - blend) + blend * wt_2)$$

Examples

RBF Example

```
import zutil

rotation = 10.0

def my_transform(x, y, z):
    v = [x, y, z]
    v = zutil.rotate_vector(v, rotation, 0.0)
    return {"v1": v[0], "v2": v[1], "v3": v[2]}

parameters = {
    ...
    "TR_1": {
        "type": "rbf",
        "zone": [4],
        "func": my_transform,
        "alpha": 200.0,
        "basis": "c2",
        "tol": 0.01,
    },
    ...
}
```

RBF Multiscale Example

```
import zutil

rotation = 10.0

def my_transform(x, y, z):
    v = [x, y, z]
    v = zutil.rotate_vector(v, rotation, 0.0)
    return {"v1": v[0], "v2": v[1], "v3": v[2]}

parameters = {
    ...
    "TR_1": {
        "type": "rbf multiscale",
        "base point fraction": 0.1,
        "zone": [4],
        "func": my_transform,
        "alpha": 200.0,
        "basis": "c2",
    },
    ...
}
```

IDW Example

```
import zutil

rotation = 10.0

def my_transform(x, y, z):
    v = [x, y, z]
    v = zutil.rotate_vector(v, rotation, 0.0)
    return {"v1": v[0], "v2": v[1], "v3": v[2]}

parameters = {
    ...
    "TR_1": {
        "type": "idw",
        "power": [4.0, 8.0, 10.0],
        "fixed zones": [1],
        "n nearest": 500,
        "deformation distance": 100.0,
        "blending stiffness": 0.5,
        "zone": [4],
        "func": my_transform,
    },
    ...
}
```

1.5.12 Overset

zCFD is capable of automatically oversetting multiple meshes into a single simulation. To run an overset case you need to provide an *override file*.

Override file

The override file tells zCFD which combinations of mesh and control dictionary to load and overset. The first entry in the list should be the background mesh, this is typically the largest of the meshes that the other meshes overlap with. The following entries in the list are then overset onto the background mesh when the solver starts. The meshes are overlapped in the order they appear in the list, starting with the background mesh.

The list should be defined in a separate python file containing an **override** dictionary.

Example **override** dictionary (e.g. override.py):

```
override = {
    'mesh_case_pair': [
        ("background_mesh.h5", "background.py"),
        ("overset_1.h5", "overset_1.py"),
        ("overset_2.h5", "overset_2.py"),
    ]
}
```

Running an overset case:

```
(zCFD)> run_zcfd -f override.py
```

Mapping

The **mapping** dictionary sets additional mapping options for overset methods and should be defined in the background control file.

Keyword	Re-quired	Default	Valid values	Description
'idw from cells order'	0	-	0 or 1	Sets the order of accuracy for IDW mapping
'number of additional overset active layers'	Yes	0	Positive integer	Adds additional active cells to overlapped mesh

Example usage:

```
parameters = {
    ..
    'mapping': {
        'idw from cells order': 0,
        'number of additional overset active layers': 0,
    }
    ..
}
```

idw from cells order

If **'idw from cells order'** is set to 0, this provides a 0th order interpolation where we only utilise data from cell a mapped point is located within. If set to 1, a first order interpolation is achieved using an IDW interpolation, using the cell a point is found in, and its neighbours.

number of additional overset active layers

Adds additional active cells which may have been made inactive by an overlapping mesh. If for example, we have a rotating domain, the resolution of the rotating boundary may result in rotated overset mesh boundary points, entering cells made inactive. This will result in no mapping between background and overset meshes at these points. To resolve this issue, it is possible to add additional active cells (for safety) to ensure a mapping between overset and background meshes. Whilst not necessary, this parameter may be useful if issues with mapping between meshes occur.

1.5.13 Write Output

write output

Controls the frequency and contents of the files output into the the **output** directory and the **VISUALISATION** subdirectory.

The **output** directory will be created in the working directory from which the solver is run and is named using the following format:

```
<case_name>_P<number of mpi ranks>_OUTPUT
```

Keyword	Required	Default	Valid values
'frequency'	Yes	Positive integer or <i>{}</i>	See " <i>frequency</i> "
'format'	Yes	'vtk'	'none' 'vtk'
'scripts'	No	[]	List of catalyst script filenames
'variable_name_alias'	No	{}	Dict
'surface variables'	Yes	["p", "T", "rho"]	List of " <i>variable</i> " names
'volume variables'	Yes	[...]	List of " <i>variable</i> " names
'volume interpolate'	No		List of surface file filenames
'fwh interpolate'	No		List of .stl file filenames
'fwh wall data'	No	False	True False
'compute average and rms'	No	False	True False
'average start time cycle'	No		Positive integer
'immersed boundary surface'	No	[]	List of dictionaries with "zone" and "stl" keys, specifying which immersed boundary zones will be mapped onto specified STL surfaces

Example usage:

```
parameters = {
  ..
  'write output' : {
    'format' : 'vtk',
    'surface variables': ['V', 'p'],
    'volume variables' : ['V', 'p'],
    'volume interpolate' : ['mesh.stl'],
    'scripts' : ['paraview_catalyst1.py'],
    'variable_name_alias' : { "V" : "VELOCITY", },
    "frequency": 500,
    'calculate average and rms': True,
    'average start time cycle': 1000,
    "immersed boundary surface": [{"zone": 7, "stl": "body.stl"},
                                  {"zone": 9, "stl": "hub.stl"}],
```

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```

    },
    ..
}

```

format

Selects the file format to output the data in. Using 'none' as format will output no files. 'vtk' outputs in vtk format for reading into [ParaView](#).

scripts

zCFD is capable of calling ParaView catalyst scripts while running, this allows you to generate "in situ" visualisation output while the solver is running.

This allows you to extract data as your simulation progresses without needing to store the full solution at every timestep. For instance a video of a slice through the dataset could be generated for an unsteady solution.

For more information about Catalyst see: <https://www.paraview.org/hpc-insitu/>

variable_name_alias

Maps the zCFD variable names to a different variable name in the output file. If downstream processes need variables named using a specific convention a naming alias dictionary can be supplied.

surface variables

A list of *variables* to output on the boundaries of the mesh. This is useful for visualisation of the flow variables on the wall of the mesh for post processing. For the 'vtk' format the surface data is written to the *output* directory with the file name:

```
<case_name>_<boundary>.pvd
```

volume variables

A list of *variables* to output in a volumetric format.

For the 'vtk' format the volume data is written to the *output* directory with the file name:

```
<case_name>.pvd
```

volume interpolate

zCFD can interpolate volume data to a supplied surface or volume mesh. This parameter lets you set a list of filenames of surfaces and/or volume meshes to interpolate to. The supported file formats are VTK (vtu or vtp files) and STL.

fwh interpolate

In addition to the 'volume interpolate' option (which outputs VTK files), zCFD is capable of writing volume interpolated data to HDF5 files for use in the *zCFD Ffowcs-Williams Hawkings (FWH) solver*. This parameter lets you list the filenames of surfaces to interpolate to for HDF5 file output. The files specifying the surfaces must be .STLs. The outputted files contain density, velocity and pressure data only, and are suitable for use as permeable surfaces in the zCFD FWH solver. The data is outputted to the *ACOUSTIC_DATA* sub-directory within the *output* directory.

fwh wall data

This parameter controls whether wall data is outputted to a HDF5 file for use in the *zCFD FWH solver*. The outputted file contains pressure data only, and is suitable for use as an impermeable surface in the zCFD FWH solver. The data is outputted to the *ACOUSTIC_DATA* sub-directory within the *output* directory.

compute average and rms

Enables computation of time averaged and RMS values for pressure, temperature and velocity. Enabling this adds these variables to the list of variables to be output automatically.

This options only applies to *unsteady* cases.

average start time cycle

If **compute average and rms** is True, this controls first real time cycle to start calculating the running average. This allows you to run the solver for a number of time cycles before you start calculating the average and RMS values.

immersed boundary surface

If the case uses immersed wall boundary conditions then force reporting on those surfaces requires STL files to be provided per immersed wall zone. The solution is interpolated onto the points in the STL so the mesh needs to be at least as fine as the boundary otherwise the accuracy of the reported forces will be affected. Additionally the normals used to calculate output values will be calculated directly from the provided STL file. Therefore a user should either use a surrogate STL generated by *zM3*, or ensure the provided STL file is watertight and has normals pointing into the body.

The interpolated solution on the STL is also output at the same frequency as other surface data.

Frequency

Sets how frequently the solver should output the flow solution. A single integer value will control output of both the volume and surface data output. A dictionary value here allows for fine grained control over the frequency with which each individual output is done. If the solver is running an unsteady simulation then this is the frequency of the real time step otherwise the pseudo cycle.

Keyword	Required	Default	Valid values
'volume data'	Yes	1.00E+08	Positive integer
'surface data'	Yes	1.00E+08	Positive integer
'volume interpolate'	Yes	1.00E+08	Positive integer
'fwf interpolate'	Yes	1.00E+08	Positive integer
'fwf wall data'	Yes	1.00E+08	Positive integer
'checkpoint'	Yes	1.00E+08	Positive integer
'volume data start'	Yes	1	Positive integer
'surface data start'	Yes	1	Positive integer
'volume interpolate start'	Yes	1	Positive integer
'fwf interpolate start'	Yes	1	Positive integer
'fwf wall data start'	Yes	1	Positive integer
'checkpoint start'	Yes	1	Positive integer

volume data, **surface data**, **volume interpolate**, **fwf interpolate**, **fwf wall data** and **checkpoint** control the frequency at which the solution data of the given type is written. The frequency is specified as the solver cycle number. The **checkpoint** option writes a *restartable* checkpoint of the flow solution at that point.

volume data start, **surface data start**, **volume interpolate start**, **fwf interpolate start**, **fwf wall data start** and **checkpoint start** specifies the first cycle that the solver should start writing that particular output.

Note

On systems with slower file I/O the overhead of writing data can slow the overall solve time, reducing the output frequency lets you address this.

Example usage:

```
parameters = {
  ..
  'write output' : {
    'format' : 'vtk',
    'surface variables': ['V','p'],
    'volume variables' : ['V','p'],
    "frequency": {
      # Output visualisation files every 3 cycles
      "volume data": 3,
      "surface data": 3,
      "volume interpolate": 3,
      "checkpoint": 3,
      # Start output every 3 cycles after 1 cycle (default = 1)
      "volume data start": 1,
      "surface data start": 1,
      "volume interpolate start": 1,
      "checkpoint start": 1,
    },
  },
  ..
}
```

1.5.14 Reporting

zCFD has the capability to output certain parameters to a <casename>_report.csv file as the solver progresses. These can be used to monitor the solver's convergence. By default, the solver outputs volume integrated residuals for each solution variable to the <casename>_report.csv file, but adding to the report dictionary means other quantities of interest can also be monitored as the simulation progresses.

Keyword	Re-quired	Default	Valid values
'frequency'	Yes	1	Positive integer
'monitor'	No	-	Dictionary of monitor point configs (MR_?)
'forces'	No	-	Dictionary of force configs (FR_?)
'massflow'	No	-	Dictionary of massflow configs (MF_?)

'frequency' sets how frequently a new line is appended to the <casename>_report.csv dictionary. If frequency = x, the solver will output to the <casename>_report.csv every x solver cycles. For a dual time-stepping simulation, this is the inner (pseudo-time), not outer, cycles.

'monitor', **'forces'** and **'massflow'** should be dictionaries of the required format. The dictionary's keys should be consecutively numbered blocks prefixed with the correct string:

Reporting on	Key name
'monitor'	MR_?
'forces'	FR_?
'massflow'	MF_?

Example usage:

For a simulation with 1000's of cycles, it can be unnecessary to report every time cycle, which slows the solver down. For a dual timestepping simulation with 20 inner time cycles, outputting every 10 cycles generally gives enough information without substantially slowing the solver down

```
# Report every 10 cycles
'report' : {
  ...
  'frequency': 10
  ...
}
```

A simulation with two monitor points and one forces block.

In addition to standard flow field outputs (see below), zCFD can provide information at monitor points in the flow domain, and integrated forces across all parallel partitions, any number of 'MR_', 'FR_' or 'MF_' blocks may be specified.

```
# Report every 10 cycles
'report' : {
  ...
  'frequency': 10
  'monitor' {
    'MR_1': {
      ...
    },
    'MR_2': {
      ...
    },
  }
  'forces' {
    'FR_1': {
      ...
    }
  }
  ...
}
```

Monitor Points

Monitor points report the specified variable at fixed mesh locations.

Keyword	Re-quired	Default	Valid values
'name'	Yes	-	String; Name of the monitor point
'point'	No	-	[x,y,z] position vector specifying a valid location in the mesh
'variables'	No	-	List of variables to report (see Output Variables)

'name' sets the name that appears in the <casename>_report.csv column heading for variables from this monitor point.

'point' should be the x,y,z location of the point of interest in the mesh as it appears in the solver (i.e. after any mesh scaling due to parameters *scaling* parameters)

'variables' controls which variables are reported at this point. In the <casename>_report.csv the column name will be a combination of the **'name'** and the variable name.

Example usage:

Tracking pressure and velocity is useful for determining shedding cycle behaviour, or in the case of a scale resolving simulation, to determine the turbulence spectrum which is being resolved. It may be important to track other variables (e.g. turbulence intensity) may also be appropriate depending on the simulation setup.

```
'report' : {
  'frequency' : 10,
  'monitor' : {
    'MR_1' : {
      'name' : 'monitor_1',
      'point' : [180.0, 100.0, 50.0],
      'variables' : ['V','p','T','Ti'],
    },
  },
},
```

Forces

Force reporting outputs the x,y,z total forces and moments on a surface or set of surfaces. These are presented as force coefficients (using the non-dimensionalisation convention used for aerofoil lift, drag and moment coefficients), as opposed to dimensional values. The force and moment coefficients resulting exclusively from viscous forces and exclusively from pressure forces are also given.

Keyword	Required	Default	Valid values	Description
'name'	Yes	–	String	Sets the name that appears in the <casename>_report.csv column headings for variables from this force monitor.
'zone'	Yes	–	List of valid mesh zone IDs (integers)	All the mesh zone IDs for the surfaces used in this force report. The forces and moments over all the zones are summed to give the forces and moments outputted in the force report.
'transform'	No	–	An (optional) transform function.	See <i>Transform function</i> . A transformation function may be supplied to the force report block to transform the force into a different coordinate system.
'reference area'	No	1	Positive number	Sets the dimensional reference area which is used to non-dimensionalise the reported force and moment coefficients
'reference length'	No	1	Positive number	Sets the dimensional reference length which is used to non-dimensionalise the moment coefficients
'reference point'	No	[0,0,0]	[x,y,z] position vector	Sets the reference point which is used to non-dimensionalise the moment coefficients
'reference pressure'	No	0.0	Positive number	For a wetted surface, this sets the pressure on the non-wetted side of the surface. Pressure forces on the surface are calculated by integrating (p - pRef) over the surface
'dimensional'	No	False	Boolean	Reports the forces in dimensional units
'inertial frame'	No	True	Boolean	Transforms the forces for rotating components into the inertial frame rather than fixed frame of original position

Example usage:

```
'report' : {
  'frequency' : 10,
  # Report force coefficient in grid axis as well as using user defined
  -transform
  'forces' : {
    'FR_1' : {
      'name' : 'force_1',
      # Required: Zones to be included
      'zone' : [1, 2, 3],
      # Transformation function
      'transform' : my_transform,
      'reference area' : 0.112032,
      'reference length' : 1.0,
      'reference point' : [0.0, 0.0, 0.0],
      # Calculate forces using a specified reference pressure
    }
  }
}
```

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```

→rather than absolute
        'reference pressure': 0.0
    },
},

```

Output names

The forces will be written into the <casename>_report.csv prefixed with the supplied **'name'**. The forces will be written with the following names:

Item	Reporting output name
Total forces and moments	'name' _F[x,y,z] and 'name' _M[x,y,z]
Forces and moments due only to pressure forces	'name' _Fp[x,y,z] and 'name' _Mp[x,y,z]
Forces and moments due only to viscous forces	'name' _Fv[x,y,z] and 'name' _Mv[x,y,z]
Transformed total forces and moments (if transform function is set)	'name' _Ft[x,y,z] and 'name' _Mt[x,y,z]
Transformed forces and moments due only to pressure forces (if transform function is set)	'name' _Ftp[x,y,z] and 'name' _Mtp[x,y,z]
Transformed Forces and moments due only to viscous forces (if transform function is set)	'name' _Ftv[x,y,z] and 'name' _Mtv[x,y,z]
Total forces and moments in static frame of reference (if specified zone is rotating)	'name' _Fif[x,y,z] and 'name' _Mif[x,y,z]
Forces and moments due only to pressure forces in static frame of reference (if specified zone is rotating)	'name' _Fifp[x,y,z] and 'name' _Mifp[x,y,z]
Forces and moments due only to viscous forces in static frame of reference (if specified zone is rotating)	'name' _Fifv[x,y,z] and 'name' _Mifv[x,y,z]

Additional information

Total force

Total force, **F**, is simply, $\mathbf{F}_p + \mathbf{F}_v$, and likewise for moments.

Non-dimensionalisation

Forces are non-dimensionalised into force coefficients as $C_x = \frac{F_x}{q_{inf}S}$ Where q_{inf} = reference dynamic pressure and S = reference area

Moments are non-dimensionalised into force coefficients as $C_{Mx} = \frac{M_x}{q_{inf}Sc}$ Where c = reference length

Dimensional pressure force

$$\mathbf{F}_p = \oint -(p - p_{ref}) \hat{\mathbf{n}} dA$$

Where p is surface pressure and $\hat{\mathbf{n}}$ is the surface normal (pointing towards the wetted area).

Dimensional viscous force

$$\mathbf{F}_v = \oint \mu \nabla \cdot \mathbf{V} dA$$

Where μ is dynamic viscosity and \mathbf{V} is the velocity vector at the wall.

Dimensional pressure moment

$$\mathbf{M}_p = \oint -(p - p_{ref}) \hat{\mathbf{n}} (x - x_{ref}) dA$$

Dimensional viscous moment

$$\mathbf{M}_p = \oint \mu \nabla V (x - x_{ref}) dA$$

Note

Reference pressure p_{ref} is dynamic pressure ($\frac{1}{2}\rho V^2$), taken from the *reference state*.

Mass flow

Keyword	Required	Default	Valid values	Description
'name'	Yes	–	String	Sets the name that appears in the <casename>_report.csv column headings for variables from this force monitor.
'zone'	Yes	–	List of valid mesh zone IDs (integers)	All the mesh zone IDs used in this mass flow monitor

'name' Sets the name that appears in the <casename>_report.csv column heading for variables from this mass flow monitor. For example, setting this to 'pipe_outflow' would mean the massflow would appear as 'pipe_outflow_massflow' in the <casename>_report.csv file

'zones' The mass flows through all the zones are summed to give a single output value for the mass flow monitor. Flow out of the domain is considered positive massflow, flow into the domain is considered positive massflow and the massflows are dimensional (typically kg per second).

Example usage:

```
'report' : {
  'frequency' : 10,
  # Report massflow ratio
  'massflow' : {
    'MF_1' : {
      # Output name
      'name' : 'massflow_1',
      # Zones to be included
      'zone' : [1, 2 ,3],
    },
  },
},
```

1.5.15 Output variables

Output Variables

Variable Name	Alias	Definition
temperature	T, t	Temperature in (K)
temperaturegrad		Temperature gradient vector
potentialtemperature		Potential temperature in (K)
pressure	p	Pressure (Pa)

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Table 1.4 – continued from previous page

Variable Name	Alias	Definition
gauge_pressure		Pressure relative to the reference value (Pa)
density	rho	Density (kg/m^3)
velocity	V, v	Velocity vector (m/s)
velocitygradient		Velocity gradient tensor
cp		Pressure coefficient
totalcp		Total pressure coefficient
mach	m	Mach number
viscosity	mu	Dynamic viscosity (Pa/s)
kinematicviscosity	nu	Kinematic viscosity (m^2/s)
vorticity		Vorticity vector ($1/s$)
Qcriterion		Q criterion
reynoldstress		Reynolds stress tensor
helicity		Helicity
enstrophy		
ek		
lesregion		
turbulenceintensity	ti	Turbulence intensity
turbulencekineticenergy		Turbulence kinetic energy (J/kg)
turbulenceeddyfrequency		Turbulence eddy frequency ($1/s$)
eddy		Eddy viscosity (Pa/s)
cell_velocity		
cellzone		
cellorder		
centre		Cell centre location
viscouslengthscale		Minimum distance between cell and its neighbours
walldist		Wall distance (m)
sponge		Sponge layer damping coefficient
menterfl		Menter SST blending function
badcells		Cells tagged as first order when using mesh quality remediation

Surface Only Quantities

Variable Name	Alias	Definition
pressureforce		Pressure component of force on a face
pressuremoment		Pressure component of moment on a face
pressuremomentx		Component of pressure moment around x axis
pressuremomenty		Component of pressure moment around y axis
pressuremomentz		Component of pressure moment around z axis
frictionforce		Skin friction component of force on a face
frictionmoment		Skin friction component of moment on a face
frictionmomentx		Component of skin friction moment around x axis
frictionmomenty		Component of skin friction moment around y axis
frictionmomentz		Component of skin friction moment around z axis
roughness		Wall roughness height
yplus		Non-dimensional wall distance
zone		Boundary zone number
cf		Skin friction coefficient
facecentre		Face centre location
frictionvelocity	ut	Friction velocity at the wall

1.6 zCFD Functions

Several parameters in the zCFD control dictionary will accept functions as arguments. These functions are then evaluated by the solver when required. This allows you to customise & tune to solver as it runs.

1.6.1 Scale Mesh Function

Description	Transform the location of a supplied point.
Valid for parameter	<i>scale_mesh</i>
Parameters	[x, y, z]: Point to transform
Returns	{'coord': [x, y, z]}: Transformed coordinates

Example:

```
# Custom function to scale z coordinate by 100
def my_scale_func(point):
    point[2] = point[2] * 100.0
    return {'coord' : point}
```

```
parameters = {
    ...
    'scale': my_scale_func
    ...
}
```

1.6.2 Transform Mesh Function

Description	Transform the location of a supplied point.
Valid for parameter	<i>mesh transform func</i>
Parameters	[x, y, z]: Point to transform
Returns	{"v1": x, "v2": y, "v3": z}: Transformed coordinates

Example:

```
rotation = 10.0

def my_transform(x, y, z):
    v = [x, y, z]
    v = zutil.rotate_vector(v, rotation, 0.0)
    return {"v1": v[0], "v2": v[1], "v3": v[2]}
```

1.6.3 Ramp CFL Function

There may be cases where more detailed control of the CFL number is desired - for example in some aerodynamic simulations where a specific physical event occurs at a given time. The CFL Ramp function lets you do this.

The ramp function returns a single floating point number (the CFL number) and can also be used to update elements of the 'cfl' Python object such as `cfl.min_cfl`, `cfl.max_cfl`, `cfl.current_cfl`, `cfl.coarse_cfl`, `cfl.transport_cfl`, `cfl.cfl_ramp`, `cfl.cfl_pmg`, or `cfl.transport_cfl_pmg`.

Description	Provide a dynamic CFL number
Valid for parameter	<i>ramp_func</i>
Parameters	<code>solve_cycle</code> , <code>real_time_cycle</code> , <code>cfl</code>
Returns	<code>cfl</code> : float

Example:

```
# Custom function to ramp CFL based on cycle, updates the cfl object variables and
→returns a CFL
def my_cfl_ramp(solve_cycle, real_time_cycle, cfl):
    cfl.min_cfl = 1.0
    cfl.max_cfl = 10.0
    cfl.cfl_ramp = 1.005
    cfl_transport = 5.0
    if solve_cycle < 500:
        cfl_new = min(cfl.min_cfl * cfl.cfl_ramp ** (max(0, solve_cycle - 1)), cfl.max_
        →cfl)
        cfl.transport_cfl = cfl_transport * cfl_new / cfl.max_cfl
        return cfl_new

    elif solve_cycle < 1000:
        cfl.transport_cfl = 7.5
        cfl.max_cfl = 15.0
        return 15.0

    else:
        cfl.transport_cfl = 10.0
        cfl.max_cfl = 30.0
        return 30.0
```

```
parameters = {
    ...
    'time marching': {
        ...
        'ramp_func': my_cfl_ramp,
        ...
    }
    ...
}
```

1.6.4 Transform Function

A transformation function may be supplied to the force report block to transform the force into a different coordinate system. This is particularly useful for reporting lift and drag, which are often rotated from the solver coordinate system.

Description	Transform a supplied point - rotate, scale or translate.
Valid for parameter	<i>Forces transform</i>
Parameters	(x, y, z): floats
Returns	(x, y, z): floats

Example:

```
#zutil is a Zenotech python library providing various utilities, available within a
-zCFD installation
import zutil

# Angle of attack
alpha = 10.0
# Transform into wind axis
def my_transform(x,y,z):
    v = [x,y,z]
    v = zutil.rotate_vector(v,alpha,0.0)
    return {v[0], v[1], v[2]}
```

1.6.5 Initialisation Function

Description	Provide the initial flow field variables on a cell-by-cell basis
Valid for parameter	<i>initial</i>
Parameters	kwargs dictionary containing “pressure”, “temperature”, “velocity”, “wall_distance”, “location”
Returns	dictionary containing one or more of “pressure”, “temperature” or “velocity”

```
def my_initialisation(**kwargs):
    # Dimensional primitive variables
    pressure = kwargs['pressure']
    temperature = kwargs['temperature']
    velocity = kwargs['velocity']
    wall_distance = kwargs['wall_distance']
    # Cell centre localtion [X, Y, Z]
    location = kwargs['location']

    if location[0] > 10.0:
        velocity[0] *= 2.0

    # Return a dictionary with user defined quantity.
    return { 'velocity' : velocity }
```

```
parameters = {
    ...
    'initial': {
        ...
        'func': my_initialisation,
        ...
    }
```

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```

    }
    ...
}

```

1.6.6 Driven initial condition

A 'driving function' provides another way of prescribing a farfield initial condition, which on evaluation returns an initial condition dictionary.

The driving function is re-evaluated at zCFD's reporting frequency, meaning that the condition (e.g. inlet velocity) can be programmed to change as the simulation progresses.

At startup, the function is only provided with the key word arguments `RealTimeStep=0`, `Cycle=0`. However, the driving function is subsequently provided with key word arguments containing all the data in the `'_report.csv'` file, evaluated at the previous timestep. For any driven initial condition, every value in the initial condition dictionary is also appended to the `_report.csv` file.

This means that the initial condition can be programmed to respond to the flow. An example is shown below, where the driven IC will continually adjust inlet angle of attack until a specified lift coefficient is achieved.

If the driven initial condition has been programmed to respond to changes in the flow, it is important to ensure that the flow has had enough time to propagate from the farfield through to the region of interest and settle before readjusting the driven initial condition. For simulations where the farfield is distant from the geometry, local and implicit time-stepping will likely give the fastest propagation of adjusted farfield conditions through the domain.

Note

Driven initial conditions **cannot** be used as reference conditions, to initialise the flow (e.g. 'IC_1') or within a restarted simulation.

Description	Provides a farfield initial condition that can respond to changes in the flow.
Valid for parameter	<i>initial condition</i>
Parameters	kwargs dictionary containing "RealTimeStep", "Cycle" and all reporting variables
Returns	dictionary containing valid keys for an <i>initial condition</i>

```

def example_ic_func(**kwargs):
    """
    Example driver function to target a lift coefficient by varying
    angle of attack
    """
    alpha_init = 0 # Initial angle of attack
    lift_target= 0.5 # Targeted lift coefficient
    update_period = 1000 # How often alpha should be updated
    flow_settling_period = 1500

    assumed_d_cL_d_alpha = 0.1 # Used to estimate alpha which would give required lift
    relaxation_factor = 1.15 # <1: under-relaxation, >1: over-relaxation

    if 'lift_target_alpha' in kwargs.keys(): # If timestep > 1
        alpha_current = kwargs['lift_target_alpha']
        F_xyz = [kwargs['wall_Fx'], kwargs['wall_Fy'], kwargs['wall_Fz']]
        F_LDS = zutil.rotate_vector(F_xyz, alpha_current, 0.0)

```

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```

lift_current = F_LDS[2] # Lift coefficient, having rotated to account for alpha
else:
    lift_current = 0 # placeholder value

if kwargs['Cycle'] < flow_settling_period:
    alpha_new = alpha_init
else:
    if (kwargs['Cycle'] % update_period) == 0:
        d_cL_required = lift_target - lift_current
        d_alpha = relaxation_factor / assumed_d_cL_d_alpha * d_cL_required
        alpha_new = alpha_current + d_alpha
        print("Alpha updated from {} to {}".format(alpha_current, alpha_new), flush_
    -= True)
    else:
        alpha_new = alpha_current

dict_out = {
    "temperature": 300,
    "pressure": 101325.0,
    'v': {
        'mach' : 0.15,
        'vector' : zutil.vector_from_angle(alpha_new, 0.0)
    },
    "reynolds no": 6.0e6,
    "eddy viscosity ratio": 1.0,
    "monitor": { # Monitor entries can be floats or lists of floats
        "prefix": "lift_target",
        "alpha": alpha_new, # Extra keys can be added to a driven IC
    -dictionary,
        "lift": lift_current, # allowing monitoring of key parameters
    -flow in the _report.csv
    },
}

return dict_out

```

```

parameters = {
    ...
    'IC_2' : example_ic_func
    ...
}

```

1.6.7 Static Pressure Ratio

The python function takes in three values (x, y, z) and returns the static pressure ratio.

Description	Returns a static pressure ratio for a given point.
Valid for parameter	<i>Static Pressure Ratio</i>
Parameters	(x, y, z): floats
Returns	float

1.6.8 Total Pressure Ratio

The python function takes in three values (x, y, z) and returns the total pressure ratio.

Description	Returns a total pressure ratio for a given point.
Valid for parameter	<i>Total Pressure Ratio</i>
Parameters	(x, y, z): floats
Returns	float

1.6.9 Total Temperature Ratio

The python function takes in three values (x, y, z) and returns the temperature pressure ratio.

Description	Returns a total temperature ratio for a given point.
Valid for parameter	<i>Total Temperature Ratio</i>
Parameters	(x, y, z): floats
Returns	float

1.6.10 Direction Vector

The python function takes in three values (x, y, z) and returns a tuple (x, y, z).

Description	Returns a direction vector for a given point.
Valid for parameter	<i>vector</i>
Parameters	(x, y, z): floats
Returns	(x, y, z): floats

```
def inflow_direction(x, y, z):
    # x, y, and z are the coordinates of the face centre
    cen = [1.0, 0.0, 0.0]
    y1 = y - cen[1]
    z1 = z - cen[2]
    rad = math.sqrt(z1*z1 + y1*y1)
    phi = math.atan2(y1,z1)
    angle = -0.24
    x2 = math.cos(angle)
    y2 = math.sin(phi) * math.sin(angle)
    z2 = math.cos(phi) * math.sin(angle)
    return (x2, y2, z2)
```

```
parameters = {
    ...
    'IC_2' : {
        'reference' : 'IC_1',
        'vector' : inflow_direction
    },
    ...
}
```

1.7 Mesh Conversion

zCFD uses unstructured meshes written in an **HDF5** file format. HDF5 provides a flexible, self describing specification supporting parallel I/O that can be tuned per filesystem type (e.g NFS, GPFS, Lustre etc).

Meshes from a wide variety of sources can be easily converted into this format as follows:

1.7.1 OpenFOAM-x.x.x

We provide a range of converters for popular mesh types via a special version of the open-source CFD code OpenFOAM, available freely for download [here](#)

Once downloaded and installed, the version of OpenFOAM will convert a range of file formats to the zCFD format. Prior to running any of these, you will need to activate your OpenFOAM environment using

```
source $FOAM_INST_DIR/OpenFOAM-x.x.x/etc/bashrc
```

1.7.2 OpenFOAM Mesh Converter

To convert from an OpenFOAM format mesh to zCFD, run the following command in the MESH directory.

```
foamTozCFD
```

This will create a new folder called *zInterface/* containing the HDF5 file.

1.7.3 Fluent Mesh Converter

The converter for **ANSYS Fluent** files is a utility called *fluent_convert*. This is included in the path set by activating the zCFD command line environment.

To run the utility, use

```
(zCFD): fluent_convert <filename>.msh <new_filename>.h5
```

or

```
(zCFD): fluent_convert <filename>.cas <new_filename>.h5
```

The will produce 2 files: the zCFD HDF5 file and the *name_zone.py* python file which holds the fluid and boundary zone names.

1.7.4 Star CCM+ Mesh Converter

There are a number of different file formats for **CD-Adapco Star CCM+** meshes. The *<filename>.sim* file is in a proprietary format and at this stage cannot be converted. The *<filename>.ccm* can be converted using

```
(zCFD): ccmconvert <filename>.ccm <new_filename>.h5
```

This produces the zCFD HDF5 file.

1.7.5 CGNS Mesh Converter

This utility will convert an unstructured, non-chimera, hexahedral mesh in CGNS (ref) format. The converter will handle meshes with element types (HEXA_8):

```
(zCFD): cgnsconvert <filename>.cgns <new_filename>.h5
```

This produces the zCFD HDF5 file. If you require support for additional element types please contact us: <mailto:zcf@zenotech.com>.

1.7.6 UGRID Mesh Converter

UGRID is a NASA format for meshes. You must follow the naming convention for UGRID files, which describes the format and *endian-ness* of the file data (“ascii8”, “b8”, “lb8”, or “r8”) depending upon which language (C or FORTRAN) was used to create the file. The mapbc file is optional and if not provided the boundary conditions of the zones default to wall.

```
(zCFD): ugridconvert <filename>.[ascii8, b8, lb8, r8].ugrid <new_filename>.h5
-><filename>.mapbc
```

This produces the zCFD HDF5 file.

1.7.7 DLR Tau Mesh Converter

Tau is a CFD solver produced by the DLR (<http://tau.dlr.de/startseite/>). Note that Tau is a node-based solver so flow field variables are calculated for and stored at the mesh nodes (or vertices) rather than at cell centres (the approach used by Star CCM+, OpenFOAM, CFX and zCFD). Thus simply converting the file format will not guarantee a good result. In many cases, the conversion will not result in a valid cell-centred zCFD mesh.

```
(zCFD): tauconvert <filename>.XXX <new_filename>.h5
```

This produces the zCFD HDF5 file.

1.7.8 SU2 Mesh Converter

SU2 is an open source CFD solver (<https://su2code.github.io/>). Note that conversion of 2D meshes is not supported as they are not handled in zCFD.

```
(zCFD): su2convert <filename>.su2 <new_filename>.h5
```

This produces the zCFD HDF5 file.

1.7.9 CBA Mesh Converter

CBA is a structured multiblock mesh format used within the University of Bristol and HMB projects. Note 2D meshes will have a symmetry plane added to extend them into 3D for use in zCFD.

```
(zCFD): cba_convert <filename>.[cba, blk] <new_filename>.h5
```

This produces the zCFD HDF5 file.

1.8 FWH solver

A Ffowcs-Williams Hawkins (FWH) solver, which is used for prediction of farfield noise, is included in the zCFD distribution. The zCFD FWH solver uses the [Farrasat 1A formulation](#), and can accept both permeable and impermeable FWH surfaces.

1.8.1 What is an FWH solver for?

A common problem in CFD is the prediction of the farfield aerodynamic noise which results from a particular airflow. Two issues make prediction of farfield aerodynamic noise challenging. First of all, many of the sources of aerodynamic noise (turbulence, vortex shedding etc.) require high fidelity, time accurate simulations and fine CFD meshes to be properly captured. Secondly, a mesh must be very fine and the simulation must have very low numerical dissipation in order to propagate aerodynamic noise any distance within a CFD mesh.

The first issue of noise simulation can be made tractable by the use of techniques like FRPM, but the second issue of far-field mesh requirements for noise propagation means that e.g. predicting the noise from a helicopter main rotor a kilometre away is simply not feasible using a conventional CFD simulation.

This issue of noise propagation in the far-field is solved by the use of the Ffowcs-Williams Hawkins (FWH) equations. These equations allow us to propagate sound to an observer an arbitrary distance away without the use of a mesh which extends all the way to the observer.

1.8.2 How does an FWH solver work?

In order to use the FWH equations to propagate noise to a far-field observer, we first run a CFD simulation and record the flow variables ($p(\mathbf{x}, t)$, $\rho(\mathbf{x}, t)$ and $\mathbf{u}(\mathbf{x}, t)$) on an ‘FWH surface’ in the near-field, noise generating region. Fig. 1.4 shows an FWH surface enclosing the nearfield for a simulation of an aerofoil in a wind tunnel.

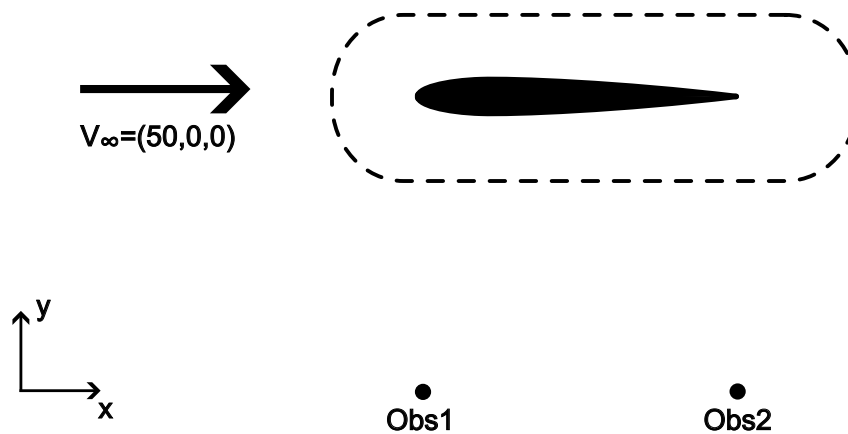


Fig. 1.4: CFD simulation of an aerofoil, including an FWH surface

The FWH surface should enclose the noise generating region, and the CFD mesh should be sufficiently fine in the near-field region to propagate noise to the FWH surface without excessive dissipation. Ideally, the FWH surface should not intersect the nearfield region of any wakes.

In some situations, it is sufficient to collect FWH surface data on the wall instead of using a separate FWH surface inside the fluid domain. FWH surfaces coincident with the wall are called *impermeable* (as opposed to *permeable*) FWH surfaces, and only require p (not p , ρ and \mathbf{u}) to be recorded.

Once the flow variables have been recorded on the FWH surface, we can propagate the noise to our observers using an FWH solver. In order to do so we must define the motion of our FWH surface and our observers in the FWH simulation. The FWH equations assume a quiescent medium (i.e. still air, with a free-stream velocity of zero), which means that the FWH surface and observer motions are frequently different to the motions used in the CFD simulation used to produce the FWH surface data.

In our example of an aerofoil in a wind tunnel, the CFD simulation has a freestream velocity, which does not satisfy the ‘quiescent medium’ condition. When using an FWH simulation to calculate the noise at the farfield observer microphone in Fig. 1.4, we therefore have to perform a co-ordinate transformation and ‘fly’ both the FWH surface and the observer microphone forwards through the quiescent medium, as in Fig. 1.5.

Once we have collected the FWH surface data from a CFD simulation and correctly defined the FWH surface and observer microphone settings, we simply use the FWH equations to propagate the pressure and velocity signals from the FWH surface to the our farfield observer locations. The equations used in the zCFD FWH solver are the [Farrasat 1A equations](#), with a retarded time formulation. The retarded time is the time τ_* at which a sound wave must be emitted by a point on the FWH surface in order for it to reach an observer at time t , given the prescribed motions of both surface and observer.

Note

The [Farrasat 1A equations](#) used by the zCFD FWH solver are only valid when the FWH surface moves through the quiescent medium subsonically. The retarded time algorithm in the FWH solver will also

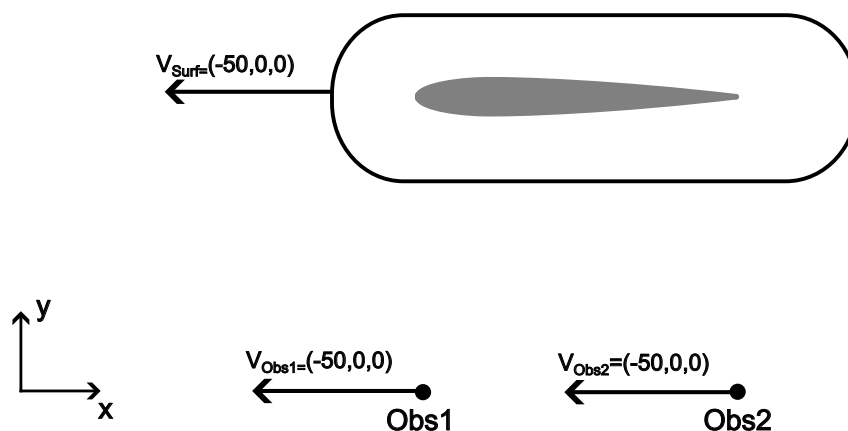


Fig. 1.5: FWH simulation of an aerofoil, with quiescent medium co-ordinate transformation applied

struggle to converge as the closing speed between an FWH surface and an observer approaches the speed of sound.

1.8.3 Running the zCFD FWH solver

There are two ways of running the zCFD FWH solver - the *fw_h python module* and the *run_fw_h utility*. The *fw_h python module* is flexible and intended for advanced users with knowledge of the python programming language. The *run_fw_h utility* is a simpler interface which requires no knowledge of the python programming language and is intended for FWH data generated using zCFD.

This documentation actually introduces the *fw_h python module* first, since doing so illustrates some mechanics of FWH solvers which all users should be aware of. The simpler *run_fw_h utility* method is subsequently introduced as an alternative, more automated method to get the same results. For a quick introduction to the zCFD FWH solver which starts with the *run_fw_h utility*, see the *FWH tutorial*.

To use the zCFD FWH solver in either format, we must first generate FWH surface data during a zCFD simulation (see *write output* for more details). The FWH surface data is stored in a HDF5 format. While no mesh conversion tools are provided, the zCFD FWH file format can easily be interrogated and replicated with tools like *h5ls* and *h5py* should you wish to convert data from other simulation tools to this format.

Using the zCFD FWH python module

The zCFD FWH solver consists of a series of python modules, which are accessible from within the *zCFD command-line environment*. Three python dictionaries, controlling the surface, observer, and solver settings, are required as inputs to the *fw_h.solve* function. This function then returns time histories of the pressures at the specified observer points, in the nested dictionaries *pOut* and *tOut*.

```
from solvers import fw_h, motion

mySurfaces = { surfaces }
myObservers = { observers }
mySolverSettings = { solverSettings }

pOut,tOut = fw_h.solve(mySurfaces, myObservers, solverSettings)
```

For an aerofoil in a wind tunnel (as in Fig. 1.4 and Fig. 1.5), an appropriate python script (including a small amount of post-processing) might look like this:

```

from solvers import fwh, motion
from matplotlib import pyplot as plt
import json

v = [-50,0,0]
surfaceCentreMotion = motion.ConstantVelocityPoint([0,0,0],v)
surfaceMotion = motion.NonrotatingSurface(surfaceCentreMotion)
obs1Motion = motion.ConstantVelocityPoint([1,0,0],v)
obs2Motion = motion.ConstantVelocityPoint([2,0,0],v)

mySurfaces = {
    "fwhSurf1": {
        "motion": surfaceMotion,
        "fileName": "./zcfdsim_P2_OUTPUT/ACOUSTIC_DATA/fwhsurf1_FWHData.h5"
    }
}

myObservers = {"Obs1": obs1Motion, "Obs2": obs2Motion}
mySolverSettings = { "c": 340, "rho0": 1.2, "p0": 1e5}

pOut,tOut = fwh.solve(mySurfaces,myObservers,solverSettings)

fig,ax = plt.subplots()
ax.plot(tOut["fwhSurf1"]["Obs1"],pOut["fwhSurf1"]["Obs1"],label="Obs1")
ax.plot(tOut["fwhSurf1"]["Obs2"],pOut["fwhSurf1"]["Obs2"],label="Obs2")
ax.set_xlabel("t (s)")
ax.set_ylabel("p (Pa)")
fig.savefig("./FWH_figure.pdf")

dataForJson = {"p": pOut, "t": tOut}
with open("./FWH_data.json","w") as f:
    json.dump(dataForJson,f)

```

When there is more than one surface, the *pOut* and *tOut* dictionaries will contain a *Surface Summation* entry in addition to the entries for each surface. This contains, for each observer, a sum of the contributions from each surface. This is useful when noise originates from several distinct regions, each covered by separate FWH surfaces (e.g. UAVs with several propellers). The *Surface Summation* entry will likely cover a shorter time period than the individual surface entries, because it only covers the time period when the observer is receiving valid noise signals from all of the FWH surfaces.

Surfaces dictionary

The zCFD FWH solver is capable of using multiple FWH surfaces in the same FWH calculation. The Surfaces dictionary therefore contains a key-value pair for each FWH surface to be used, where the key is the surface's name (to be used in the FWH solver) and the value is an *individual surface definition dictionary*. The surface name must be a string, and cannot be 'Surface Summation'.

Example usage:

```

from solvers import motion
v = [-50,0,0]
surfaceCentreMotion = motion.ConstantVelocityPoint([0,0,0],v)
surfaceMotion = motion.NonrotatingSurface(surfaceCentreMotion)

mySurfaces = {
    "fwhSurf1": {

```

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```

    "motion": surfaceMotion,
    "fileName": "./zcfdsim_P2_OUTPUT/ACOUSTIC_DATA/fwhsurf1_FWHData.h5"
}
}

```

Individual surface definition dictionary

Keyword	Required	Default	Valid values	Description
'motion'	Yes		A <i>surface motion class</i>	The motion of the surface through the FWH medium
'fileName'	Yes		A readable file path	The FWH surface data, in the FWH HDF5 format outputted by the zCFD solver
'permeable'	No	Automatically deduced from the FWH surface data file	True False	Whether or not the surface is permeable or not (see <i>above</i>).
'flipSurfaceNormals'	No	False	True False	Whether or not to invert the FWH surface normals before running the FWH solver. The surface normals should always point outwards towards the farfield. For FWH surface data generated using the <i>fwf interpolate</i> keyword in the zCFD solver, the surface normal direction depends on the .stl file used to define the FWH surface, and can be checked using a visualisation tool (e.g. Paraview).
'transformSurfaceVelocity'	No	True	True False	Relevant for permeable surfaces only, and should normally be kept <i>True</i> . Setting this to <i>False</i> means that the FWH surface fluid velocity used in the FWH solver does not include the velocity resulting from the motion of the surface (as defined by the 'motion' keyword above). This option may be required when using data from other solvers, in the case where the FWH surface moves through a quiescent medium during the simulation used to create the FWH surface data.

Observers dictionary

The Observers dictionary defines a list of observer microphones at which farfield noise should be calculated. In the observers dictionary, keys are used to set the observer's name in the FWH solver output, and the value sets the motion of the observer. Observer motions must be defined using the *point motion classes*.

Example usage:

```

from solvers import motion
v = [-50,0,0]
obs1Motion = motion.ConstantVelocityPoint([1,0,0],v)
obs2Motion = motion.ConstantVelocityPoint([2,0,0],v)

myObservers = {"Obs1": obs1Motion, "Obs2": obs2Motion}

```

Solver settings dictionary

The solver settings dictionary sets the properties of the FWH medium, and the numerical settings used in the FWH solver.

Example usage:

```
mySolverSettings = { "c": 340, "rho0": 1.2, "p0": 1e5}
```

Keyword	Required	Default	Valid values	Description
'c'	Yes		Positive number	speed of sound in the far-field medium, m/s
'rho0'	Yes		Positive number	density of the far-field medium, kg/s
'p0'	Yes		Positive number	static pressure of the far-field medium, Pa
'dt'	No	set equal to the smallest timestep between outputs in all the FWH surface data files specified in the <i>surfaces dictionary</i>	Positive number	timestep between observer microphone recording times, s
'breakToIAbs'	No	'dt' set in the solver settings dictionary / 1000	Positive number	the time accuracy (s) with which we would like to predict the retarded time τ_* in the retarded time calculation.
'maxIts'	No	50	Positive integer	The maximum number of iterations to use in the algorithm used to predict retarded time
'observer-StartTime'	No		Number	The simulation time (s) at which observers start recording data. If this is not set, this will be set automatically to be the earliest time when a surface/observer pair has a valid signal.
'ob-serverEnd-Time'	No		Number	The simulation time (s) at which observers end recording data. If this is not set, this will be set automatically to be the last time when a surface/observer pair has a valid signal.

Point (observer) motion classes

FWH Observers are points which move through the FWH quiescent medium according to the function $x = f(t)$. In the zCFD FWH solver, we define the motion of observers using one of the following classes, which are available inside the *solvers.motion* module inside the zCFD command line environment (see *above*).

Motion Class	Inputs	Description
<i>OriginPoint()</i>		A point which is always on the origin, i.e. $f(t) = [0, 0, 0]$.
<i>StationaryPoint(X0)</i>	X0: a 3-d vector $[x0, y0, z0]$	A point which is stationary, i.e. $f(t) = [x0, y0, z0]$.
<i>ConstantVelocityPoint(X0,dXdt)</i>	X0: a 3-d vector $[x0, y0, z0]$ dXdt: a 3-d vector $[dxdt, dydt, dzdt]$	A point with constant velocity, i.e. $f(t) = [x0 + t * dxdt, y0 + t * dydt, z0 + t * dzdt]$

Surface motion classes

Just like FWH Observers, FWH Surfaces require their motion to be defined. There are two surface motion classes - NonrotatingSurface and RotatingSurface. Both use a *point motion class* to define the motion of their 'centre point'. In this way, complex motions like that of a propellor which is both rotating and translating through the FWH medium can be defined.

Motion Class	Inputs	Description
<i>NonrotatingSurface(centrePoint)</i>	centrePoint: a <i>point motion class</i>	A surface which does not rotate, and translates at the same velocity as the 'centrePoint'.
<i>RotatingSurface(centrePoint,axis,omega)</i>	centrePoint: a <i>point motion class</i> axis: a 3-d vector $[ax_x, ax_y, ax_z]$ omega: a number.	A surface which translates at the same velocity as the <i>centrePoint</i> , and also rotates about the centre-Point with rotation axis <i>axis</i> and rotation angular velocity (rad / s) <i>omega</i>

Using the zCFD run_fw utility

When using the *fw python module* defined above, we manually define FWH *surface*, *observer* and *solver settings* dictionaries which are used in *fw.solve()*. This gives us fine grained control, but for most FWH simulations which are based on zCFD CFD simulations, the input dictionaries to *fw.solve()* can actually be generated automatically by reading the *zCFD input parameters file*. This is what the *run_fw* utility does. Within the *zCFD command-line environment*, the *run_fw* utility can be called as below:

```
run_fw -c <zcfid control file> --reference_condition <reference condition>
--observer_locations <observers .csv file>
```

The *run_fw* utility reads the *zcfid control file* and the *observers .csv file*, and based on these, automatically runs the FWH solver. Assuming the *zcfid control file* input was *zcfidSim.py* and the *observers .csv file* specified the observers *Obs1* and *Obs2*, the *run_fw* utility would:

1. automatically generate the inputs to the *fw.solve()* function, setting the observer and surface motions based on the *reference condition* and using all FWH surfaces that the CFD simulation defined by *zcfidSim.py* outputs
2. Run the *fw.solve()* function, saving the screen output to *zcfidSim.fwh.log*
3. Save the sum of the contributions of all FWH surfaces at the observers *Obs1* and *Obs2* to the *.csv* files *zcfidSim.fwh.Obs1.csv* and *zcfidSim.fwh.Obs2.csv* respectively.

For the example outlined in the *fw python module example*, the *run_fw* command would look something like this:

```
run_fw -c zcfidSim.py --reference_condition IC_1 --observer_locations observers.csv
```

zCFD control file

The first input to the `run_fwh` utility is the *zCFD control file*. This is the control file for the zCFD simulation which generated the FWH surface data files which are to be used. For the example outlined in [Fig. 1.4](#) and the *fwh python module example*, the *zCFD control file* would be called `zcfdsim.py` and would look something like the example below.

```
parameters = {
    ...
    "IC_1": {
        "temperature": 288,
        "pressure": 1e5,
        "V": {"vector": [50,0,0]},
        ...
    },
    ...
    "write output": {
        ...
        "fwh interpolate": ["fwhsurf1.stl"],
        ...
    },
    ...
}
```

The `run_fwh` utility reads the zCFD parameter file and finds the paths to all the FWH surface output files which were generated by the zCFD CFD simulation defined by `zcfdsim.py`. In this case, it would find the file `./zcfdsim_P2_OUTPUT/ACOUSTIC_DATA/fwhsurf1_FWHData.h5`.

Reference condition

In the *fwh python module example*, we have to manually define the solver settings and the motions of the observers and surfaces through the FWH quiescent medium manually. However, if all the surfaces and observers are in the same *translational reference frame*, we can set the motions and solver settings directly from a zCFD *IC block*.

Being in the same *translational reference frame* means that all the surfaces and observers translate through the FWH quiescent medium at the same velocity. In practice, this means that all observers are *static* in the ‘mesh’ frame of reference, i.e. do not ‘fly by’. [Fig. 1.4](#) and [Fig. 1.5](#) show that for the example, *Obs1*, *Obs2* and the FWH surface are in the same translational reference frame, hence can be used in the `run_fwh` utility.

In the example case, we would set our reference frame to be *IC_1*. This is the freestream conditions in the `zcfdsim.py` CFD simulation. The pressure and temperature in *IC_1* set the `c`, `p0` and `rho0` in the *solverSettings dictionary*. The velocity in *IC_1* sets the motion of our surfaces and observers through the FWH quiescent medium. Since *IC_1* defines a freestream velocity of `[50,0,0]`, our surface and observers move through the FWH quiescent medium at a velocity of `[-50,0,0]`, just as in [Fig. 1.4](#) and [Fig. 1.5](#).

In most cases, a zCFD simulation control file will already contain an IC block suitable for use as the `run_fwh` reference condition. Since zCFD control files can contain unused IC blocks, simply add a suitable IC block to the zCFD control file if one does not already exist.

Which *translational reference frame* an FWH surface is in is independent of whether the FWH surface is rotating or not - see [below](#) for more details.

Observer .csv file

In the `Observers.csv` file, we define the locations of the observers (in the ‘mesh fixed’ frame of reference). To match the observers shown in [Fig. 1.4](#) and [Fig. 1.5](#), the *observers.csv* file should contain the following:

```
Obs1, 1.0, 0.0, 0.0
Obs2, 2.0, 0.0, 0.0
```

Advanced use

The `run_fwh` utility allows and accounts for *overset* zCFD simulations and FWH surfaces which exist in zCFD *rotating fluid zones*. This means that even complex simulations like drones with multiple rotating propellers can be simulated with the `run_fwh` utility.

Where the input *zCFD control file* is an *overset 'override' file*, FWH surfaces from all control files specified in the override dictionary are used and the reference condition (e.g. `IC_1`) is taken from the first control file specified in the override dictionary. Where FWH surfaces exist in *rotating fluid zones*, the surfaces remain in the same *translational reference frame* as the observers, but also rotate as specified in the rotating fluid zone specification.

The `run_fwh` utility does not allow translating meshes or translational boundary conditions, since both would introduce ambiguity into what the correct *translational reference frame* for the FWH surfaces and observers should be. As explained *above*, 'fly-by' observers are also not possible in the `run_fwh` utility.

In the *fwh python module*, `fwh.solve()` outputs the contribution from each individual FWH surfaces to each observer pressure history, as well as the sum of all contributions. The `run_fwh` utility only records the sum of contributions from all FWH surfaces in the output `.csv` files. This means that in the `run_fwh` utility, all noise generating noises in the zCFD simulation are implicitly assumed to be enclosed by single FWH surfaces. This means that, for instance, including both *fwh interpolate* and *fwh wall data* FWH surface data output in a zCFD control file is likely to lead to double accounting in the `run_fwh` utility.

Where the `run_fwh` utility is not suitable, it is still possible to use components of the `run_fwh` utility to automate parts of a *fwh python module* workflow. A simplified summary of what happens within the `run_fwh` executable is detailed below, showing the use of the *fwh_helper_functions* which can be used in the *fwh python module* to automate workflows.

```
from solvers import fwh_helper_functions
rho0, p0, c, freestreamV = fwh_helper_functions.get_zcf_ref_conditions(
    "zcfSim.py", "IC_1"
)
surfaces = fwh_helper_functions.get_zcf_surfaces(
    "zcfSim.py", freestreamV
)
observers = fwh_helper_functions.get_csv_observers(
    "observers.csv", freestreamV
)
solverSettings = {"rho": rho0, "p0": p0, "c": c}
pOut, tOut = fwh.solve(surfaces, observers, solverSettings)
fwh_helper_functions.write_fwh_data_to_zcf_csv("zcfSim.py", tOut, pOut)
```

1.8.4 FWH file utilities

As well as the FWH solver itself, two FWH file utilities are provided - *writeFWHSurfaceFrequenciesFile* and *writeBlankedOffFWHSurfaceFile*. Users may find these utilities useful for investigating the sources of noise within their CFD simulation.

writeFWHSurfaceFrequenciesFile

This python function takes an FWH surface file as input, and creates a file where the FWH surface data can be viewed in the frequency, instead of time, domain.

This can be useful for visually indicating where particular frequencies originate from in an FWH observer pressure signal. To generate the FWH surface frequencies file, an FFT (using a Hann window) of the FWH data is calculated at each surface face. The data stored in the surface frequencies file at a particular surface face and chosen frequency is then the magnitude of that FFT's amplitude, at the chosen frequency. The data can be viewed by opening the `.xdmf` file corresponding to the output file in Paraview - the 'time' chosen in Paraview corresponds to the frequency being viewed. The data at frequency = 0 corresponds to the time average of the FWH surface data.

Example usage:

```
from solvers import fileManipulation
fileManipulation.writeFWHSurfaceFrequenciesFile("./myFWHSurface.h5",
"./myFWHSurface_
-Frequencies.h5")
```

writeBlankedOffFWHSurfaceFile

This python function writes a copy of an FWH surface file where specified faces are ignored by the FWH solver. Sometimes it is useful to ‘blank off’ certain areas from an FWH surface output file before the FWH solver is run - for example, if CFD setup constraints mean the noise from that region of the FWH surface is non-physical and should therefore be ignored when calculating FWH noise data. This function takes an input FWH surface file, copies it to an output FWH surface file, then sets to zero the face area of any face in the output file where the python function shouldBlankOff(x,y,z) returns ‘True’ for the face’s (x,y,z) co-ordinates. When the face area of a face has been artificially set to 0, that face will not contribute to the observer location pressures calculated by the FWH solver. The region which has been set to have 0 face area can be inspected visually by opening the *.xdmf* corresponding to the output file in Paraview

Example usage:

```
from solvers import fileManipulation

def isPositiveX(x: float, y: float, z: float):
    if x > 0:
        return True
    else:
        return False

fileManipulation.writeBlankedOffFWHSurfaceFile("./myFWHSurface.h5",
"./myFWHSurface_
-IgnorePositiveX.h5", isPositiveX)
```

1.9 zM3

zM3 or “zMesh Cubed” is a mesh generator that is included in the zCFD distribution. It is a general purpose meshing tool that can rapidly create cut cell cartesian, or immersed boundary meshes for zCFD’s finite volume solver. As a user you define the domain and can then include geometry in the form of STL files to include in the domain. Mesh refinement can be controlled in a number of ways including explicit refinement regions as well as refinement based on the size of the STL triangulation.

1.9.1 Execution

zM3 is included in the standard zCFD installation, to run it simply activate your zCFD environment in the normal way and the *zm3* executable will be added to your path.

```
zm3
```

To see the command line options run:

```
zm3 -help
```


1.9.2 Options

Option	De- fault	Description	Example
<code>-meshName</code>	mesh	String defining the output mesh name	<code>-meshName output.h5</code>
<code>-base</code>	0 0 0	Three real numbers defining the (min_x, min_y, min_z) corner	<code>-base 0.0 0.0 0.0</code>
<code>-dims</code>	1.0 1.0 1.0	Three real numbers defining the x, y, z extent of the domain	<code>-dims 100.0 100.0 100.0</code>
<code>-globalSpacing</code>	1.0	Real number defining largest cell size in the mesh	<code>-globalSpacing 5.0</code>
<code>-stlFiles</code>		List of STL files containing surfaces for meshing	<code>-stlFiles file1.stl file2.stl</code>
<code>-stlSpacing</code>		Target cell size for each STL surface file loaded, the the same order as specified in <i>stlFiles</i>	<code>-stlSpacing 1.0 0.5</code>
<code>-relativeSpacings</code>	0 (for each STL)	Integer for each STL file specified, 1 = True, 0 = False. If True then the spacings defined in <i>stlSpacing</i> are treated as a factor multiplying the local STL size to get the spacing value at that location.	<code>-relativeSpacings 0 1</code>
<code>-minSurfaceSpacing</code>		Minimum surface spacing when using <i>relativeSpacings</i>	<code>-minSurfaceSpacing 0.5</code>
<code>-maxSurfaceSpacing</code>		Maximum surface spacing when using <i>relativeSpacings</i>	<code>-maxSurfaceSpacing 0.5</code>
<code>-generateSurrogateSTL</code>		Integer list specifying which STL files should be have a surrogate STL generated on them. Indexing begins at 0.	<code>-generateSurrogateSTL 0 2</code>
<code>-includeProximitySpacings</code>	0 (for each STL)	Integer for each STL file specified, 1 = True, 0 = False. If True reduce cell sizes to account for the proximity of other triangles nearby.	<code>-includeProximitySpacings 0 1</code>
<code>-refineAnisotropicSTLTris</code>	0 (for each STL)	Integer for each STL file specified, 1 = True, 0 = False. If True triangles will be sub-divided until all edges approach the smallest edge length for that STL.	<code>-refineAnisotropicSTLTris 0 1</code>
<code>-includeCutCells</code>	0	Integer specifying if cells intersected by STL are to remain in mesh, 1 = True, 0 = False	<code>-includeCutCells 1</code>
<code>-seedPoints</code>		List of three real numbers defining a point in the mesh to be kept, from which flood filling occurs. Multiple seed points can be defined.	<code>-seedPoints 50.0 50.0 50.0</code>
<code>-solidPoints</code>		Three real numbers defining a point in the mesh, within a region which must be deleted. Defines non-fluid regions. Multiple solid points can be defined.	<code>-solidPoints 10.0 5.0 3.0</code>
<code>-boxRefinement</code>		Lists of 7 real numbers defining a refinement box in the order x_min y_min z_min x_max y_max z_max spacing.	<code>-boxRefinement 20.0 20.0 20.0 50.0 50.0 50.0 7.5</code>
<code>-surfaceBoxRefinement</code>		Similar to <i>boxRefinement</i> but only STL elements within the box will be given the target refinement.	<code>-surfaceBoxRefinement 20.0 20.0 20.0 50.0 50.0 50.0 7.5</code>

1.9. zM3

<code>-rotatedTranslatedRefinement</code>		A rotated and translated box refinement region. The box is rotated around 0,0,0 and then translated. The rotation is defined by	<code>-rotatedTranslatedRefinement 10.0 10.0 10.0 0.0 0.0 1.0 10.0 10.0 10.0 7.5 75</code>
---	--	---	--

1.10 Visualisation

zCFD by default will output data in **VTK** format. This format can be read directly by many post-processing tools including **ParaView** by Kitware.

Output in other formats is also possible, including **TECPLOT** and **EnSight** as follows:

1.10.1 VTK Output

By default, zCFD will output data in VTK format. To explicitly force VTK output, use the following option in the *'write output'* part of the control dictionary:

```
'write output' : {  
    # Output format  
    'format' : 'vtk',
```

1.10.2 EnSight Output

To output in EnSight format, use the following option in the *'write output'* part of the control dictionary:

```
'write output' : {  
    # Output format  
    'format' : 'ensight',
```

1.10.3 Native HDF5 Output

To output in HDF5 format (the native format for zCFD), use the following option in the *'write output'* part of the control dictionary:

```
'write output' : {  
    # Output format  
    'format' : 'native',
```

1.10.4 ParaView Catalyst Scripts

ParaView provides a powerful yet lightweight interface that allows parallel processing of simulation data during programme execution called **ParaView Catalyst**. This is driven by scripts (Python files) that can be called when data is output:

```
'write output' : {  
    # Output format MUST be VTK  
    'format' : 'vtk',  
    # The scripts should be in the same directory as the input files  
    'scripts' : ['paraview_catalyst1.py', 'paraview_catalyst2.py']
```

1.10.5 ParaView Client

To download the free ParaView software for visualising VTK format data on the local device, just visit the [Paraview website](#).

1.10.6 ParaView Client-Server

In addition to running entirely locally on a device, ParaView can interface to a remote server. This allows users to run ParaView to access data that is held (and processed) on a different computer, potentially running larger simulation tasks that would be possible on the local machine. This also means that there is no need to transfer the large output files back to a local machine for post-processing. The remote machine can easily be set up to run a ParaView Server in parallel - meaning that very large post-processing jobs can be run quickly.

ParaView Server

To download and install ParaView Server, you can either use the version on the main ParaView website and follow the instructions [here](#).

Alternatively or else use the version bundled with zCFD. The 'pvserver' included in the zCFD distribution includes plugins for reading the zCFD HDF5 mesh format directly.

To start a ParaView Server on your computer within the zCFD environment run:

```
> pvserver
```

ParaViewConnect

`ParaviewConnect` is a helper utility for connecting to remote ParaView servers. It reduces the complexity of setting up the required ssh connections and works well with zCFD. More information and installation instructions can be found on the [Github page](#).

1.10.7 ParaView Post-Processing Best Practices for Parallel zCFD Data

When post-processing solution data generated in parallel by zCFD using ParaView, it is important to understand the differences between various ParaView filters and their impact on data interpolation. This section provides guidance on recommended pipelines for accurate results.

CleantoGrid vs MergeBlocks

Two commonly used ParaView filters for processing parallel datasets are **CleantoGrid** and **MergeBlocks**. Each has distinct characteristics:

CleantoGrid Filter:

- **Purpose:** Merges points that are exactly coincident and removes degenerate cells
- **Interpolation:** Performs minimal interpolation, preserving original data values at cell centres and vertices
- **Use case:** Recommended when data accuracy is critical and you want to preserve the original computed values
- **Characteristics:** May result in slightly fragmented visualisations at block boundaries but maintains data fidelity

MergeBlocks Filter:

- **Purpose:** Combines multiple blocks into a single unstructured grid
- **Interpolation:** May perform interpolation across block boundaries to create smooth transitions
- **Use case:** Better for smooth visualisations and streamline generation across block boundaries
- **Characteristics:** Creates visually smoother results but may alter original computed values through interpolation

Recommended Pipelines

For **quantitative analysis** and **data extraction** (probes, line plots, force calculations):

```
# Recommended pipeline for quantitative analysis
import paraview.simple as pvs

# Load data
reader = pvs.PVDReader(FileName='solution.pvd')

# Use CleantoGrid to preserve data accuracy
clean_data = pvs.CleantoGrid(Input=reader)
```

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```
# Convert to point data if needed
point_data = pvs.CellDatatoPointData(Input=clean_data)

# Proceed with analysis (probes, calculators, etc.)
```

For **visualisation purposes** (streamlines, contours, volume rendering):

```
# Pipeline for smooth visualisations
import paraview.simple as pvs

# Load data
reader = pvs.PVDRReader(FileName='solution.pvd')

# Use MergeBlocks for smoother visualisations
merged_data = pvs.MergeBlocks(Input=reader)

# Convert to point data for smooth contouring
point_data = pvs.CellDatatoPointData(Input=merged_data)

# Apply visualisation filters (streamlines, contours, etc.)
```

Important Considerations

1. **Data Accuracy:** Always use CleanToGrid when extracting quantitative data for analysis or validation
2. **visualisation Quality:** MergeBlocks may provide better visual results for presentations and general visualisation
3. **Performance:** CleanToGrid is typically faster as it performs less processing
4. **Block Boundaries:** Be aware that different filters may show artefacts differently at parallel decomposition boundaries
5. **Regression Testing:** When comparing results across different runs, ensure consistent filter usage

Example Notebook Usage

The following pattern is recommended in Jupyter notebooks when processing zCFD parallel data:

```
import paraview.simple as pvs

# For data extraction and analysis
def load_for_analysis(filename):
    reader = pvs.PVDRReader(FileName=filename)
    reader.UpdatePipeline()
    clean = pvs.CleanToGrid(Input=reader)
    return clean

# For visualisation and rendering
def load_for_visualisation(filename):
    reader = pvs.PVDRReader(FileName=filename)
    reader.UpdatePipeline()
    merged = pvs.MergeBlocks(Input=reader)
    point_data = pvs.CellDatatoPointData(Input=merged)
    return point_data
```

This ensures that your analysis maintains data integrity while your visualisations remain smooth and professional.

1.10.8 Jupyter Notebooks

We also recommend the use of [Jupyter Lab](#) for post-processing zCFD runs. This is one of the easiest ways to use Python, via an interactive notebook on your local computer. The notebook is a locally hosted server that you can access via a web-browser. Jupyter is included in the zCFD distribution and notebooks for visualising the residual data will automatically be created when you run a zCFD case. In addition there are several example notebooks available in the [zPost](#).

To automatically start up notebook server on your computer within the zCFD environment run:

```
> start_lab
```

1.11 Utilities

zCFD is bundled with a number of utility functions to streamline specific workflows:

1.11.1 Actuator disc modelling

Overview

When simulating the effects of an aerodynamic force device (such as a wind turbine or propellor) on flow field, it is often impractical to resolve the flow down to the scale of the blades. Instead the effects of the device on the flow can be represented using an actuator disc model, which is then superimposed into the flow as a set of additional source terms.

Actuator disc definitions

Conceptually turbines and propellers behave nearly identically in terms of the actuator disc model, with the only differences being in the coordinate systems and sign conventions typically used to define them. In zCFD an actuator disc zone is defined as a fluid zone, using the following keys:

```
turb_zone = {
  "FZ_1": {
    "type": "disc",
    "controller": {},
    "geometry": {},
    "discretisation": {},
    "model": {},
    "name": "turbine_name",
    "reference plane": True,
    "def": "./turbine_vtp/turbine_def.vtp",
    "reference point": [x, y, z],
    "update frequency": 1,
  }
}
```

The *controller* dictionary defines how the forces generated from the disc should be controlled. Options here are *fixed* and *tsr curve*. For a fixed controller the user must specify an angular velocity and blade pitch angle, and for a tsr curve the user must specify a tip speed ratio curve, and optionally a blade pitch curve in the case of a *BET* model.

```
"controller": {
  "type": "tsr curve",
  "tip speed ratio": tsr,
  "tip speed ratio curve": [
    [u0, tsr0],
    ...
    [un, tsrn]
```

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```

    ],
  },
  "controller": {
    "type": "fixed",
    "omega": omega,
    "pitch": pitch
  },
},

```

The *geometry* dictionary contains the physical description of the disc geometry, and has the following keys:

```

"geometry": {
  "centre": [x, y, z],
  "inner radius": inner_radius,
  "normal": [x, y, z],
  "outer radius": outer_radius,
  "up": [x, y, z],
},

```

Here the *normal* direction will determine the direction of force from the disc. The convention in zCFD is that the normal should point on the direction of the force on the fluid. i.e. for a propeller the normal should point in the direction of the flow, and on a turbine it should point towards the incoming flow.

The *discretisation* dictionary contains the information needed to create the actuator disc representation of the turbine/ propellor:

```

"discretisation": {"type": "disc", "number of elements": 48},

```

The *model* dictionary contains the information needed to drive the force calculation in the actuator disc model. Here the user can specify either a *simple* turbine model, which averages the performance of the turbine over the entire disc, or *BET* to use a blade element model:

```

"model": {
  "type": "simple",
  "kind": "turbine",
  "power model": "curve",
  "thrust coefficient": thrust_coefficient,
  "thrust coefficient curve": [
    [u0, tc0],
    ...
    [un, tcn]
  ],
  "power": turbine_power,
  "turbine power curve": [
    [u0, p0],
    ...
    [un, pn]
  ],
},

"model": {
  "type": "BET",
  "kind": "propellor",
  "blade chord": [
    [r0/R, c0],
    ...
    [1.0, cn],

```

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```

],
"blade twist": [
  [r0/R, t0],
  ...
  [1.0, tn],
],
"number of sections": 24,
"number of blades": 2,
"aerofoil positions": [[0.0, "aerofoil1"], [1.0, "aerofoil1"]],
"aerofoils": {
  "aerofoil1": {
    "cd": [
      [a0, cd0],
      ...
      [an, cdn],
    ],
    "cl": [
      [a0, cl0],
      ...
      [an, cln],
    ],
  },
  ...
},
"tip loss correction radius": 0.8,
"tip loss correction": "rstar",
},

```

1.12 Troubleshooting

CFD solvers can sometimes fail to converge or even crash when running. zCFD includes an automatic validation to ensure that the inputs are consistent and syntactically correct, and there are some common problems that can be identified even if the code has crashed.

1.12.1 Crashing

There are several common causes of code crashing:

1. Numerical instability
2. Inconsistent boundary conditions
3. Preconditioning
4. Poor mesh quality

Numerical instability

The solver will try to advance the flow solution towards convergence at the required level of spatial and temporal accuracy, subject to a user-defined limit called the *CFL* (Courant–Friedrichs–Lewy) number. The CFL number limits the update to the solution in each cycle to maintain the stability of the underlying numerical scheme.

There are formal criteria for the CFL number for given schemes, however these typically only apply to idealised (orthogonal or structured meshes with very gradual variation in cell-to-cell volume ratios). For complex meshes or where cell quality may be poor (even in only a few cells), the limit for stability may be significantly less. In explicit mode, the theoretical CFL limit is formally approximately 1.0 for most schemes - though in many cases a higher value (1.5 to 2.0) will actually work. In implicit mode the CFL limit is theoretically 1000 or more, with values between 10 and 100 quite common.

The solver will provide some feedback as it is running that can be helpful in diagnosing stability issues.

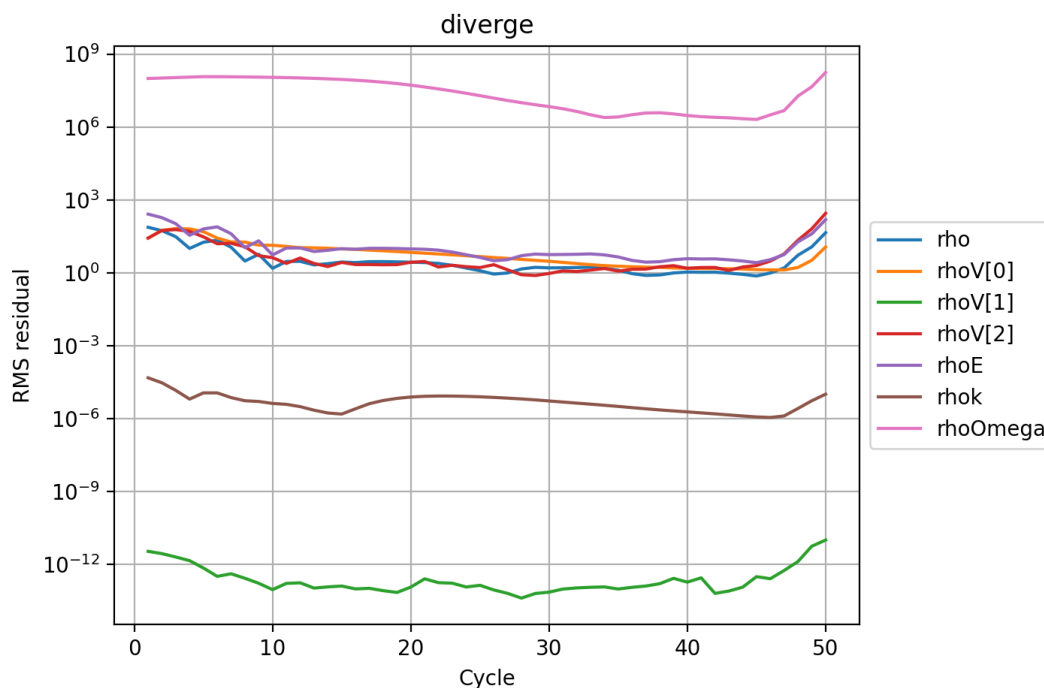


Fig. 1.6: The typical form of a divergent set of residuals. Rather than decreasing, the values all start increasing significantly from cycle 45 onwards. In this case the NACA0012 case was deliberately set with an unstable explicit CFL number of 6.0.

The residuals that are output in the `_report.csv` file should gradually reduce as the solver converges (per real time step if the flow is unsteady). If one or more of the reported values starts diverging, there is a good chance that the scheme has become unsteady. Note that this can also be a consequence of a particular pattern in the flow that appears during the solution process and so this divergence may occur after a period of otherwise stable convergence. For *implicit* runs using the AMGX library, reporting includes the number of cycles of the implicit linear solver and the residual value associated with each. Typically 4 to 5 cycles should be enough. If the number of iterations to achieve the desired improvement in accuracy (typically 3 to 4 orders of magnitude) starts increasing above 6, then the underlying linear system may be poorly conditioned, which will be due to numerical instability in the solution.

Listing 1.1: Example output from the AMGX implicit linear solver. In this case the turbulence equations are solved after the primary flow variables. The primary flow variables are solved in 5 cycles of the AMGX solver, achieving an order of magnitude 3 reduction in the residuals.

```
Cycle 5003 (real time cycle: 0 time: 0)
CFL 20.0 (20.0) - MG 20.0 (coarse mesh: 0)
iter      Mem Usage (GB)      residual      rate
-----
Ini              36.9899      3.037596e-06
0              36.9899      4.565379e-07      0.1503
1              36.9899      1.138337e-07      0.2493
2              36.9899      3.056741e-08      0.2685
3              36.9899      1.061114e-08      0.3471
4              36.9899      3.308933e-09      0.3118
5              36.9899      1.293730e-09      0.3910
```

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```

-----
Total Iterations: 6
Avg Convergence Rate:      0.2743
Final Residual:            1.293730e-09
Total Reduction in Residual: 4.259057e-04
Maximum Memory Usage:     36.990 GB
-----
Total Time: 0.869665
  setup: 0.109454 s
  solve: 0.760211 s
  solve(per iteration): 0.126702 s
  iter      Mem Usage (GB)      residual      rate
-----
    Ini          36.9899    1.713350e-04
    0           36.9899    1.060694e-07    0.0006
    1           36.9899    1.898567e-10    0.0018
-----
Total Iterations: 2
Avg Convergence Rate:      0.0011
Final Residual:            1.898567e-10
Total Reduction in Residual: 1.108102e-06
Maximum Memory Usage:     36.990 GB
-----

```

If the solver is crashing due to numerical instability, it may be worth reducing the *CFL* number to less than 1.0 (say 0.5) for explicit mode or 5.0 (or less) for implicit mode. The spatial *'order'* can also be reduced to 'first' and the *'inviscid flux scheme'* to 'Rusanov' (the most stable, though least accurate discretisation scheme).

If the solver still crashes, then the problem is likely to be due to an issue with the boundary conditions, pre-conditioning or the mesh quality.

Wall functions

zCFD includes a useful feature to automatically scale a turbulent wall function on a solid boundary. This is implemented via an internal iterative solution of a set of equations to match the flow speed and the wall shear stress in the cell adjacent to the wall, according to the ideal profile of a turbulent boundary layer. The number of internal iterations should be quite low (less than 20) if the solution is physically valid. zCFD reports on the time per cycle, and if this value starts climbing it may indicate that the wall function iterations are not converging. To test whether the wall functions are causing problems, switch the type of the *boundary condition* from 'wallfunction' to either 'slip' or 'noslip' depending upon which is a closer approximation to the desired behaviour.

Inconsistent boundary conditions

zCFD will automatically check whether boundary conditions BC_* in the input file are correctly specified, but it cannot determine whether a combination of boundary conditions is correct. For example a closed fluid domain (all boundary conditions set to solid wall) except for a single mass flow condition will initially start converging until the pressure either rises or falls to non-physical levels. The effects of mismatched boundary conditions can also be more subtle - especially with inflow and outflow conditions resulting in over-specification or under-specification of the solution.

A good way to diagnose inconsistent boundary conditions is to remove complexity and simplify the boundary conditions (e.g. replace wall functions with slip conditions, inflow and outflow conditions with Riemann farfield conditions). It can also be helpful to repeat the simulation, deliberately stopping the solver just before the crash in order to inspect the solution for unexpected features. Inspection of the 'temperature' values in a solution can often point to areas of the flow that are causing problems. This is particularly the case when poor quality cells are present.

Preconditioning

The timestep for zCFD running in explicit mode is limited by a local numerical wave-speed in the solver scheme. In regions of low speed flow (such as near stagnation points) this may be overly conservative. Preconditioning is used to modify the scheme to increase the local timestep subject to a local stability condition. However, the stability limits of the preconditioned scheme may be inappropriate for a given mesh, leading to flow field divergence. The easiest way to test this is to set *'precondition'* to False in the solver scheme settings.

Parallel log files

Note that for parallel runs, the main log file may not contain all of the information relating to a crash where the solution on a particular partition has caused the problem. The log files for each partition are stored in the `_OUTPUT/LOGGING` directory as `.<partition>.log`.

1.12.2 Convergence stall

More common than crashing is convergence stall - where the reported residuals initially reduce and then plateau.

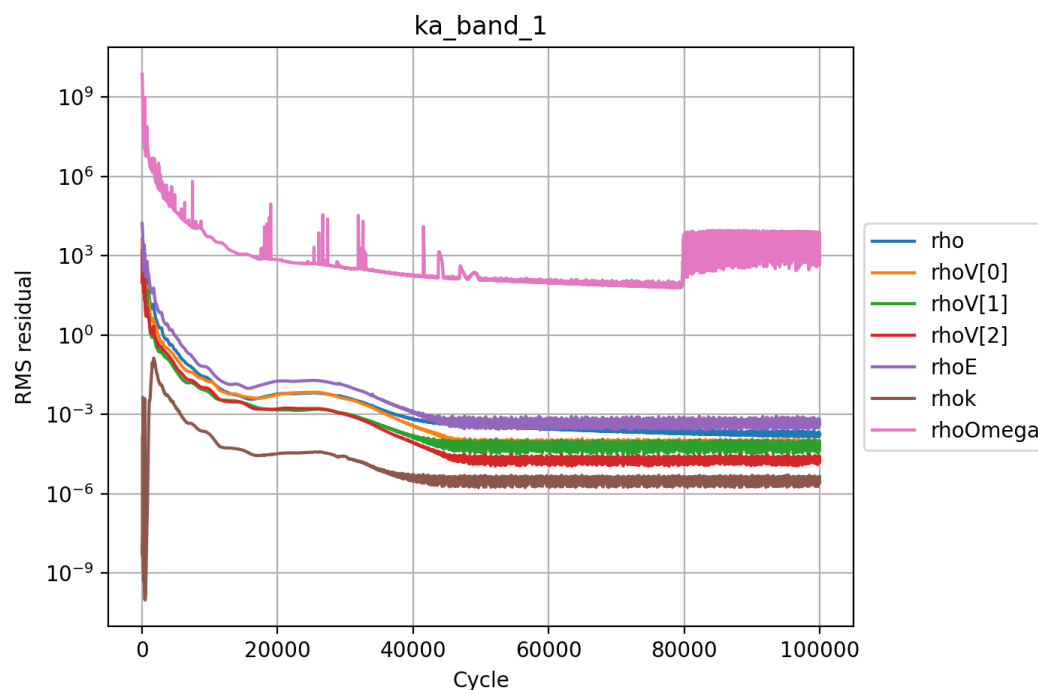


Fig. 1.7: The convergence of the steady-state explicit solver has achieved an average residual reduction of 5 orders of magnitude and then stalled. The noise in the solution from 40k cycles onwards suggests that either the flow is not fundamentally steady-state or that multigrid is adding an error to the solution. The user must determine whether the level of convergence is sufficient for their purposes and if not whether to run an unsteady simulation or degrade the spatial accuracy.

There are several common causes of convergence stall:

1. Multigrid
2. Flow unsteadiness

Multigrid

For explicit simulations, the use of *multigrid* will accelerate the convergence of the solver by using a set of coarse meshes to propagate longer wavelength solution components faster through the domain than would be possible on the finest mesh, subject to the CFL condition. In theory, and for idealised meshes, the use of multigrid does not change the steady-state solution (or pseudo-steady-state solution for unsteady flows) that is reached. However for real meshes around complex geometry, multigrid does introduce an error and this can effectively limit convergence. The use of the keyword 'multigrid cycles' in the 'time marching' section of the control dictionary will turn off multigrid after a specified number of cycles to remove this error.

Flow unsteadiness

A very common cause of convergence stall - particularly for steady-state simulations is due to physical unsteadiness in the underlying flow. In such cases, the solver is attempting to find a steady-state solution to an unsteady problem and the result is that the solution keeps changing in each iterative cycle. There are two approaches to dealing with this - depending upon the flow features of interest.

If the unsteadiness is important then the unconverged steady-state flow can be used as the starting point for an unsteady simulation. If the convergence stall is within the pseudo-steady cycles of an unsteady dual time-stepping solution, then it may be that the physical *time step* specified is too large and should be reduced.

On the other hand, if the unsteadiness is not of interest then the accuracy of the solution can be deliberately degraded to provide a more 'average' steady-state flow. This might include using the Rusanov inviscid flux scheme, switching the spatial accuracy to first order and / or using a coarser mesh. Note that the implicit mode of the solver can also be used to filter the solution in time as larger time-steps can be achieved with a higher CFL number. The user should note that this approach can cause solver instability and inaccuracy in the final solution, as the 'averaging' process is non-physical.

It may also be the case that the flow residuals are stalled, but the integrated properties of interest (e.g. lift, drag, mass flow) are sufficiently converged as to be useful. This decision is left to the user.