ACSE 9 IRP: Project Plan

Duncan Hunter

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Supervisor: Dr. A. Obeyesekara

1 Rationale and Project Objectives

Pipe and pipe network flow analysis is an important real world problem in areas such as water distribution and refining. The computational fluid dynamics (CFD) code ICFERST (*Pain et al.*, 2001; *Gomes et al.*, 2017; *Salinas et al.*, 2017a,b) can simulate turbulent flows, yet understanding the ICFERST workflow is a barrier for its use. This project aims to make the cumbersome process of generating meshes for ICFERST easier, and to automate the ICFERST workflow for pipe/pipe network flow analyses.

The software produced in this project has several requirements to meet the project's objectives. It needs to have the ability to create specific pipe network geometries (e.g. an engineer could specify a design, or batches of designs) easily, that are compatible with ICFERST. Geometrical information from meshes needs to be passed from the pre-processing software to ICFERST and the post-processing software, as part of automating the workflow of conducting analyses of one or several pipes/pipe networks.

If there is time in the project, optimisation of pipe networks could be developed, using the post-processing results of multiple simulations to reach an optimum. The software should be able to run on a high performance computer (HPC). This reduces the time taken for simulations significantly and is critical in determining whether optimisation is possible.

The desired entire process is shown in Figure 1, with information being passed between different pieces of software to create a more automatic process. An engineer could start at either a low or high level: an engineer without detailed knowledge could conduct flow analyses easily, but also a developer could create further tools, and both have an easy process conducting a pipe flow analyses.

2 Literature Review

2.1 ICFERST

ICFERST uses control volume finite element methods with adaptive meshing to simulate fluid flow, with either single or multiphase flow, as well as porous media flow. *Gomes et al.* (2017) describe ICFERST as allowing continuous and discontinuous descriptions of inter-element pressure and saturation, as well as have arbitrarily high-order polynomial representations for velocity and pressure. Mesh adaptivity, not used in many commercial CFD codes, is key as it can increase accuracy in areas of high complexity,

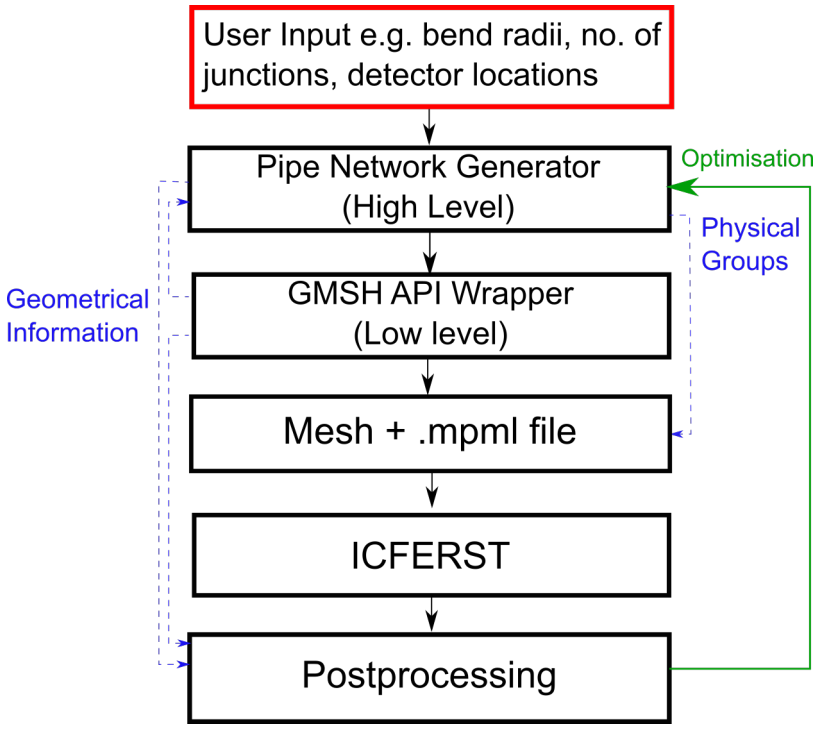

Figure 1: Ideal ICFERST process post project completion. Blue dashed lines show the passing of information between softwares. Green shows the optimisation loop.

as found often in turbulent flow. It can allow the user to not need to know a priori the areas of mesh-refinement. *Pain et al.* (2001) details how ICFERST attempts to optimise and adapt a mesh. It visits each element in the mesh, and performs a several different operations to alter the local area. Then if one of the operations improves the output of a functional related to the size and shape of the element, and meets other specific requirements, then the change is accepted. Otherwise, it is marked to not be visited again in a sweep, so as to save computational time. This process can involve creating elements, which can improve the resolution of the simulation in complex areas.

2.2 Mesh Generation

Before using any CFD code, meshes need to be generated to specify the domain, and the initial and boundary conditions. This project aims to build on an existing meshing software to create tools. The GMSH-API (*Geuzaine and Remacle*, 2009) has been chosen for the following reasons: it uses Python (but could also use Julia or C++); it is code based, rather than graphical user interface (GUI) based; it can interface with ICFERST's requirement for *Physical Groups*; and can create specific, complex objects. Python is ideal as it is a commonly used programming language, and has useful built-in functionality. Being code based is critical, as this project hopes to produce software that can be used on HPCs, and built on by this project's pipe generators and potential optimiser. *Physical groups*, used commonly in GMSH, are needed to define initial and boundary conditions in ICFERST, which already has compatibility for GMSH files. The ability to create complex and specific geometries is critical, as it allows engineers to recreate designs accurately for analyses. GMSH contains features from OpenCASCADE, which allows it to create complex objects such as junctions and mitered bends through boolean operations such as fuse and intersect.

There are many softwares available, but the project is limited by ICFERST's ability to use GMSH

style meshes. Potential softwares reviewed that could have been used include SALOME (*Ribes and Caremoli*, 2007) or PyGMSH, which adds raw GMSH code to a file. It was found that these all had downsides greater than any found in the GMSH-API. For example, SALOME would require developing a tool to convert files to a format acceptable to ICFERST, and did not have obvious physical groups. Furthermore, the OpenCASCADE features it uses appear to be included in the GMSH-API. PyGMSH was found to be outdated and not as powerful as the GMSH-API. GMSH is also open source, and while it is supported primarily by one person, it is still updated regularly.

2.3 Pipe flow

Problems of turbulent flow in pipe bends are studied often, as they can be useful in determining how effective a pipe is, and how much wear the pipe will endure. An early analysis of pipe flow in a sharp bend is from *Tunstall and Harvey* (1968). A good introduction and analysis of turbulent pipe flow in smooth bends can be found in *Hufnagel* (2016), where swirl switching is analysed. *Sierra-Espinosa et al.* (2000a,b) and *Sakowitz et al.* (2014) have conducted analyses of junction flow. The tools this project will make creating geometries for these analyses easier, and may lead to more complex analyses. The cited analyses could be used as test cases.

2.4 Optimisation

Optimisation could involve creating and evaluating (by simulation, rather than modelling) many meshes, and generating fitness scores from post-processing results. Algorithms for optimizing pipe networks include genetic algorithms (*Dandy et al.*, 1996) and memetic algorithms (*Eusuff and Lansey*, 2003). These approaches are for large networks using more simple models than full simulation of turbulent flow. There may not be enough time or computing power for this project to optimise pipe networks using turbulent flow simulations.

3 Proposed Approach and Prototype Program

This project aims to write code that can be used at both a high and low level, as in Figure 1. A GMSH-API wrapper will be low level, and will be used in a pipe/pipe-network generator which should be high level and easy to use.

3.1 GMSH Wrapper and Pipe Generator

Class based wrappers will be created, creating GMSH entities and storing useful and easy to access properties of GMSH entities, as well as useful functions. Many of these properties (examples listed below), are geometrical, and are often hard to access and manage when writing with the GMSH-API (or GMSH alone). Examples of entities that could be created include cylinders, smooth bends, mitered bends, and junctions.

- Location
- Direction
- GMSH dimensions
- Centre of faces
- Direction of faces
- Radius[1]
- Centre of object
- GMSH tags
- Length[1]

[1]Where applicable

An example pseudocode of a GMSH entity is in Listing 1.

Listing 1: Cylinder class example with example functions.

```
class Cylinder():
        def __init__(self, properties of cylinder):
                self.properties = properties
                gmsh.create_object(properties of cylinder)
                if direction:
                        gmsh.rotate()
                if position:
                        gmsh.translate()
        self.update_properties()
        def rotate(self, new_direction, centre_of_rotation):
            gmsh.rotate()
            self.update_properties()
        def fuse(self, object):
            gmsh.fuse()
        def update_properties(self)
            self.properties = new_properties
```

Pipes or pipe networks could then be created in a modular, sequential fashion; either manually at a low level by using these classes (demonstrated in Figure 2), or the high level pipe/pipe network generator could be used. This would involve the engineer giving rules or requirements to the software, which then creates the pieces automatically through the GMSH-API wrapper. Rules could be simple, such as exits being 10 diameters from a curve, or more complex, perhaps involving multiple junctions.

3.2 ICFERST workflow and automation

The pipe generator should be able to pass geometrical data (such as locations of entries and exits of pipes) to ICFERST as well as post-processing software. As this data will be stored in python classes, it should be easy to access. The generator could also store information about the surfaces of the pipe, such as which one is the inlet, outlet or wall. This is useful as it can be passed to ICFERST as physical groups. Ideally, this could lead to using python and regular expressions to automatically generate the .mpml file (an xml style file with properties of the simulation) needed for simulations. If this is done, then the automated process of using ICFERST is greatly enhanced. This .mpml file contains many options, but many will often be the same, or could be automatically calculated. For example, the boundary conditions are likely to be no-slip for the walls, and zero pressure for the outlet. The maximum number of elements created from mesh adaptivity could be found from the size of the mesh created and applying a simple relationship (e.g. if the mesh has x elements, the maximum number of elements is yx).

3.3 Optimisation

A simple genetic algorithm could be developed to optimise small pipe networks at first, and if time permitting, larger networks. This would likely involve using a physical attribute such as velocity or pressure from post-processing to create a fitness score for a network. This may not be feasible, as running simulations is time consuming, and genetic algorithms typically involve running many hundreds of possible configurations.

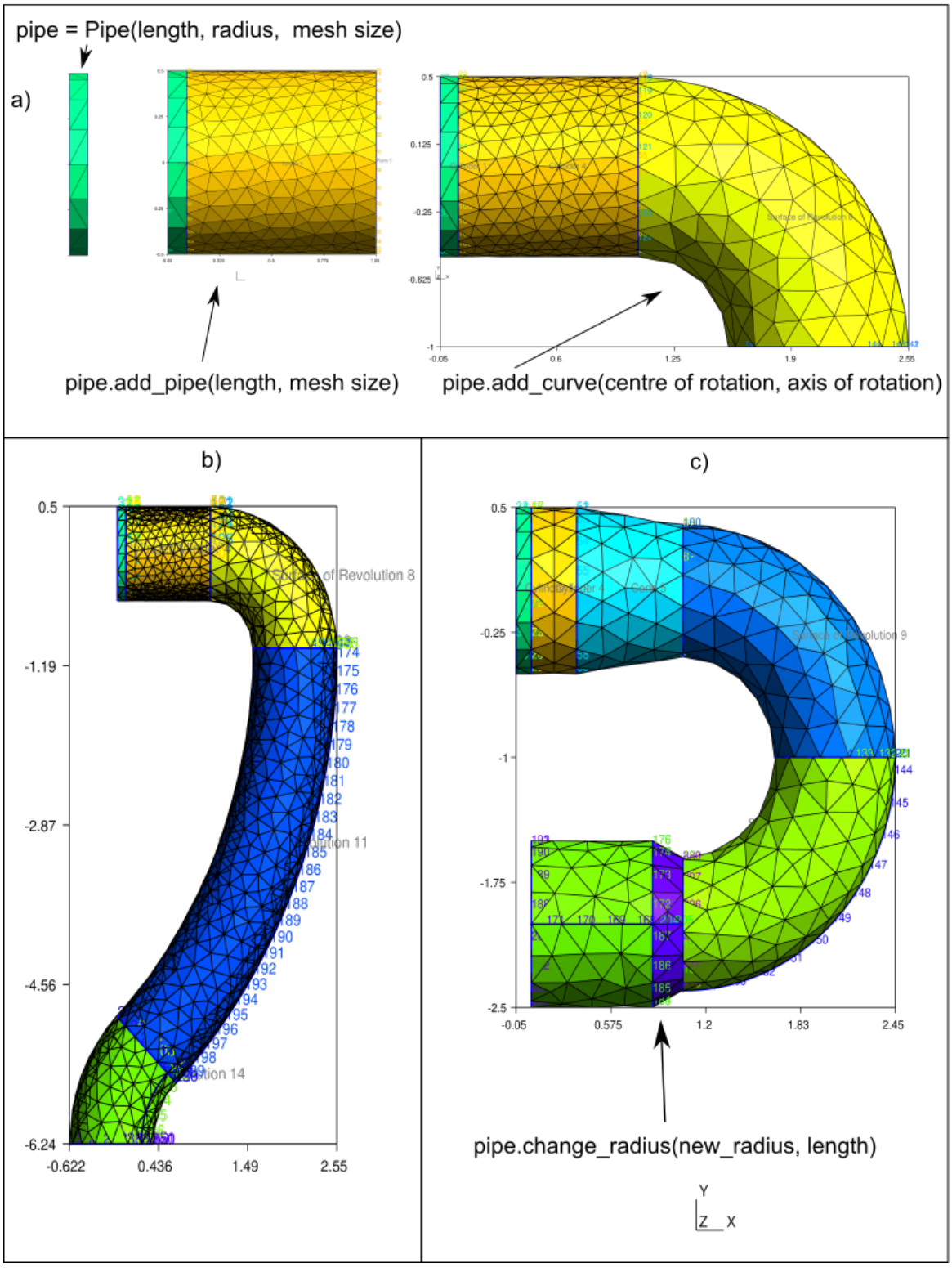

Figure 2: An early prototype, showing that specific geometries can be created. a) Sequential, modular pipe building. b) Arbitrary radii can be created. Curves can specified by 3 dimensional vectors representing x, y and z and by the centre of rotation. c) Radius of pipe can be changed.

Figure 3: Gantt chart showing ideal project timeline

3.4 Code Sustainability

If possible, TravisCI will be used to perform continuous integration. It may not work perfectly, as Travis may not be able to use some of the libraries this project uses (such as GMSH-API). If so, then test scripts will be written that can be executed locally. Documentation will be written during development, both to ease the process of writing new software that builds on previous work, and to improve the quality (as freshly written code is easier to understand). Documentation will be in the form of doc-strings, and a LaTeX manual. Ideally, parts of this project could be uploaded to PyPI, so users can easily install it using pip-install.

4 Deliverables and deadlines

The timeline of this project is in Figure 3. There are three main phases of development: the GMSH-API wrapper, the pipe-network generator, and optimisation. There is time left at the end to focus on the report, and fix any bugs and clean up code. A test case could be created for each prototype, allowing test-driven development. As the project will build on and modify earlier created tools, it is important to maintain functionality.

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