Coiled tube reactors under pulsed flow conditions have been shown to demonstrate promising mixing behavior. Optimizing the geometry and operating conditions of coiled tube reactors is important to investigate performance, identify underlying physics and ensure industrial feasibility. Experiments and computational studies have verified that by encouraging radial mixing, and discouraging axial mixing, coiled tube reactors under pulsed flow conditions promote plug-flow performance which enables tighter product distributions [3, 8, 9, 11, 12]. Computational fluid dynamics (CFD) simulations of the system are expensive due to complex vortex phenomena, and gradient information is unavailable. The resulting expensive black-box optimization problem is analogous to hyper-parameter optimization [1, 4, 7, 14]. However, chemical discovery [5, 10], and engineering design [2, 6, 13] are also examples of domains where expensive black-box optimization problems are formulated. For example as follows

$$x^* = \underset{x \in \mathcal{X} \subset \mathbb{R}^d}{\operatorname{argmax}} f(x). \tag{1}$$

In this coursework you will optimise a 2D approximation to a coiled tube reactor system using a machine learning optimisation method of your choice. An example simulation is shown in Figure 1. Make note that

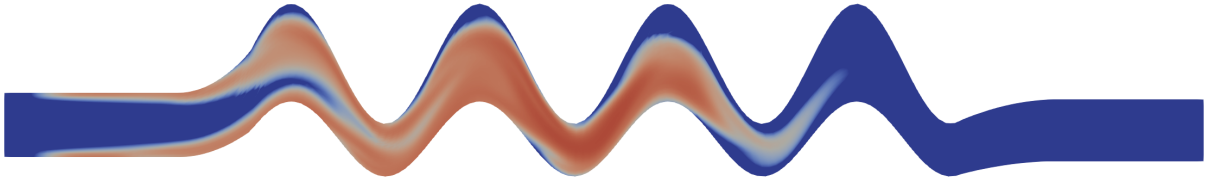


Figure 1: An example simulation.

CFD simulations of the reactor are computationally expensive, and take on the order of 10 minutes. Therefore, you will have to be careful about how many points you sample, and where.

1 System Description

1.1 Parameterisation

The reactor is parameterised by five values: amplitude of pulsed-flow, frequency of pulsed-flow, and three geometry parameters. Examples of reactor geometries and solutions **will not be given**, and we encourage groups to investigate these themselves. This is to encourage the use of machine learning to explore the search space as opposed to attempting to heuristically locate an optimal solution. Table 1 shows the upper and lower bounds for all five parameters.

Table 1: Lower and upper bounds of problem parameters

Parameter	**Lower bound**	**Upper bound**
Amplitude of pulsed-flow	0.001	0.008
Frequency of pulsed-flow	2	8
Geometry parameter 1	0.1	0.7
Geometry parameter 2	3	6
Geometry parameter 3	0	$\pi/2$

1.2 Inside the black-box

The simulation has been set up in such a way that you will only need to provide a set of parameters and the function will return a value which represents the plug-flow performance. **You should not modify this code**. However, in the interest of transparency the following procedures are performed.

1. A folder is created within `outputs/` that is named after the datetime the function is evaluated. This folder will contain all information about a given simulation.

2. Reactor geometry is created from the given parameters, and a preview is saved to the folder, named `reactor_geometry.png`. Subsequently, geometry is then meshed into finite elements.
3. A simulation is then performed in `OpenFOAM` via the `PyFoam` library using the given operating conditions.
4. From the concentration profile that is returned at the outlet of the reactor, a dimensionless number is calculated which represents plug-flow performance.

2 Getting Started

2.1 Instructions

The following process has been set up for you as a way to run CFD simulations on your own computer. Note that whilst this seems long winded: be patient, and read all the steps. This is significantly easier than installing OpenFOAM and all the relevant libraries yourself.

1. Download and install Docker by clicking here and following the instructions.
2. In a terminal, and in the desired location, clone the Git repository. For example in my Documents folder:

```
$ cd Documents
$ git clone https://github.com/OptiMaL-PSE-Lab/ml_coursework.git
```

   If Git is not installed, download and install Git by clicking here and following the instructions.

3. Then enter the Git repository:

```
$ cd ml_coursework
```

4. Build the Docker image:

```
$ docker build --no-cache -t ml_coursework .
```

5. Run the Docker image as a container. This will also enable all the output files to be shared with your host machine.
   - **If you are on Mac or Linux run the following command:**

```
$ docker run -v $(pwd)/:/root/ml_coursework/ -it -p 8888:8888 ml_coursework
```

   - **If you are in the Windows terminal run the following command:**

```
$ docker run -v /cd/:/root/ml_coursework/ -it -p 8888:8888 ml_coursework
```

6. You should now be within the Docker container and should see something ending in `#`. Here enter the following command to start a Jupyter notebook.

```
# jupyter notebook --ip 0.0.0.0 --port 8888 --no-browser --allow-root
```

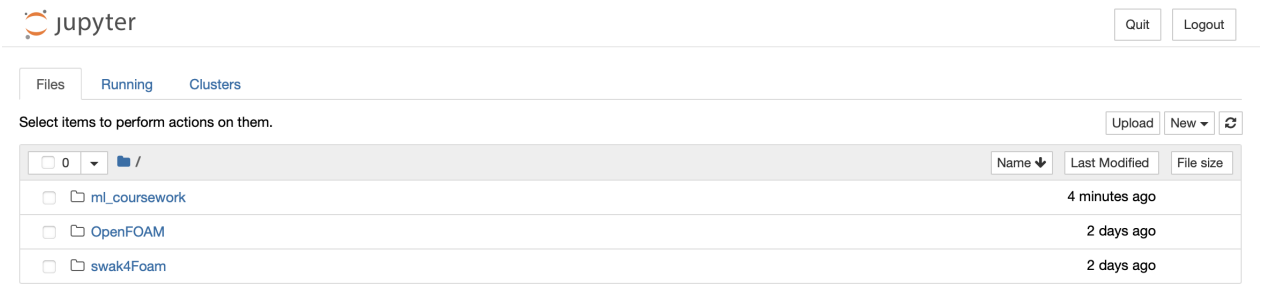
7. The terminal will then prompt you with

```
    To access the notebook, open this file in a browser:
      file:///root/.local/share/jupyter/runtime/nbserver-640-open.html
Or copy and paste one of these URLs:
     http://41b527251408:8888/?token=044321e3fdb7493b611b493d...
 or http://127.0.0.1:8888/?token=044321e3fdb7493b611b493d80d23...
```

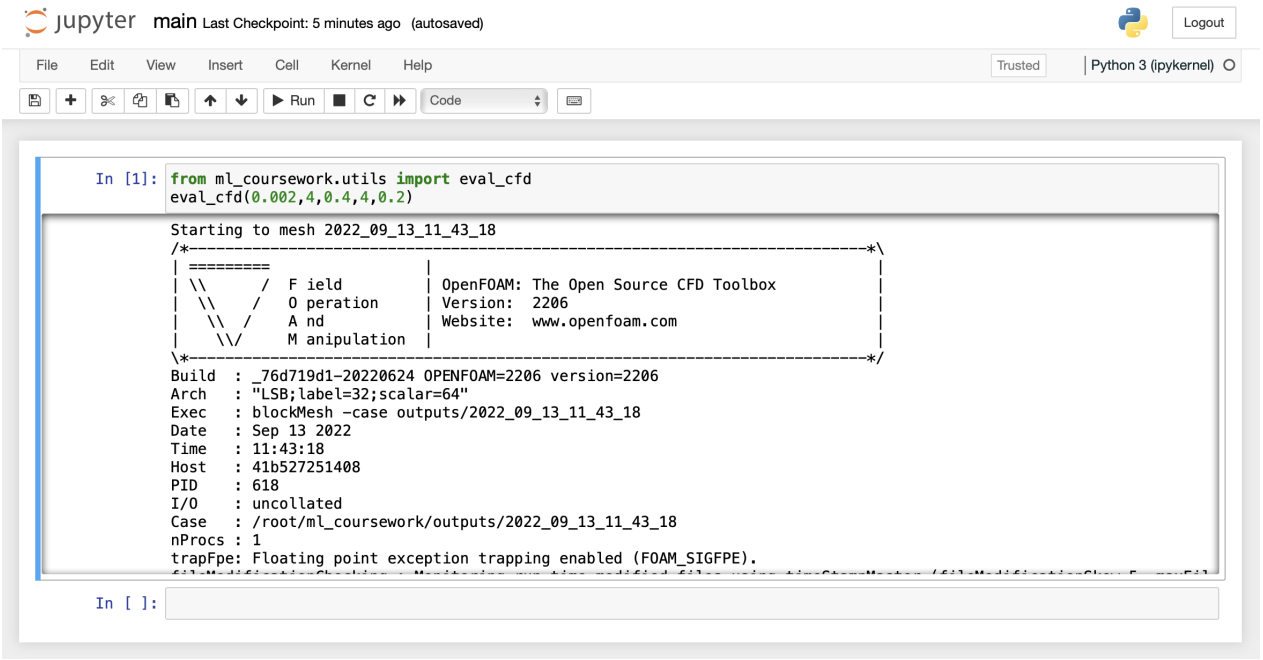
   I prefer to use the last URL which I copy and paste into my browser. Note these URLs are just examples that I have generated and they will not work for your machine.

2.2 Jupyter Interface

In your browser you should now see the following



If you enter the `ml_coursework` folder you will find everything you need, mainly the `main.ipynb` file. If you click on this file you will find the single function which evaluates the CFD code. If you run the cell, the output should look something like this:



To check the simulation is running properly, check in the folder where you cloned the Git repository. The a folder containing this simulation

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