



Reduced Order Modelling, Simulation and Optimization of Coupled systems

Validation of Fluid-Structure Interaction Simulations in Membrane-Based Blood Pumps

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Abstract

the proposed benchmark can be used for training in the fields of mathematical modeling of a coupled system, model testing and error estimation.

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List of Acronyms

| | |
|---------------|---|
| ITMATI | Technological Institute of Industrial Mathematics |
| FSI | Fluid-Structure Interaction |
| ITMATI | Technological Institute of Industrial Mathematics |
| LVAD | Left Ventricular Assist Devices |
| XFEM | Extended Finite Element Method |
| WMBP | Wave Membrane Blood Pumps |

1. Introduction

Wave Membrane Blood Pumps (WMBP) [1], developed at CorWave SA, may represent the new frontier of Left Ventricular Assist Devices (LVAD). The pumping technology of WMBP is based on the wave undulations of an immersed elastic membrane that propels the blood against an adverse pressure gradient, from the left ventricle into the ascending aorta. In Figure 1, left, we show the cross sectional view of the pump device.

The intertwined dynamics in WMBP are studied in the framework of Fluid-Structure Interaction (FSI) modeling and solved in the mathematical domain shown in Figure 1, right. Blood is modeled as a viscous incompressible Newtonian fluid with density ρ_f and viscosity μ_f , by means of Navier-Stokes Equations. The wave membrane Ω_1^s is considered a linear material at small deformations, according with previous publication [2], with density ρ_s^1 and Lamé parameters λ_s^1 and μ_s^1 . The same holds for the magnet ring Ω_2^s , with parameters ρ_s^2 , λ_s^2 and μ_s^2 . For sake of simplicity, we combine structure properties in unique space-dependante variables, e.g. $\tilde{\rho}_s(\mathbf{x}) = \rho_s^1$ if $\mathbf{x} \in \Omega_1^s$, and $\tilde{\rho}_s(\mathbf{x}) = \rho_s^2$ if $\mathbf{x} \in \Omega_2^s$. Hence, the formulation of the problem is the following: for each time $t > 0$, find fluid velocity and pressure $(\mathbf{u}(t), p(t))$ in the fluid domain $\Omega^f(t)$ and structures displacement $\hat{\mathbf{d}}(t)$ in the reference structure domain $\hat{\Omega}^s = \Omega^s(0) = \Omega_1^s(0) \cup \Omega_2^s(0)$, such that:

$$\rho_f (\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}) - \nabla \cdot \mathbf{T}^f(\mathbf{u}, p) = \mathbf{0} \quad \text{in } \Omega^f(\mathbf{d}), \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega^f(\mathbf{d}), \quad (2)$$

$$\tilde{\rho}_s \partial_{tt} \hat{\mathbf{d}} - \nabla \cdot \hat{\mathbf{T}}^s(\hat{\mathbf{d}}) = \mathbf{0} \quad \text{in } \hat{\Omega}^s, \quad (3)$$

$$\mathbf{u} = \partial_t \hat{\mathbf{d}} \quad \text{on } \Sigma(\mathbf{d}), \quad (4)$$

$$\mathbf{T}^f(\mathbf{u}, p) \mathbf{n} = \mathbf{T}^s(\hat{\mathbf{d}}) \mathbf{n} \quad \text{on } \Sigma(\mathbf{d}). \quad (5)$$

where $\mathbf{T}^f(\mathbf{u}, p) = -p\mathbf{I} + 2\mu_f \mathbf{D}(\mathbf{u})$, with $\mathbf{D}(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$, is the fluid Cauchy stress tensor and $\hat{\mathbf{T}}^s(\hat{\mathbf{d}}) = \tilde{\lambda}_s (\nabla \cdot \hat{\mathbf{d}}) \mathbf{I} + 2\tilde{\mu}_s \hat{\mathbf{D}}(\hat{\mathbf{d}})$ is first Piola-Kirchhoff structure tensor. Notice that the fluid domain Ω_f and the interface Σ depend over time on structure displacement \mathbf{d} (geometric coupling). Physical coupling conditions (4) and (5) guarantee the continuity of velocity and of stresses at the fluid-structure interface Σ , respectively.

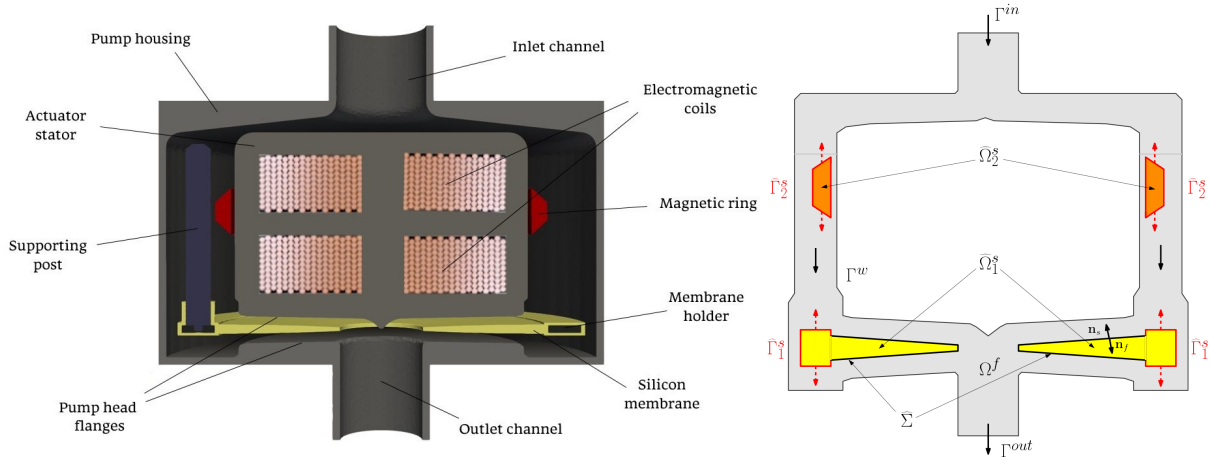


Figure 1: Left: Cross section of wave membrane blood pumps. The blood enters from the inlet channel, it flows down along the sides of the central actuator body, it interacts with the wave silicon membrane and it is finally ejected into the outlet channel. Membrane vibrations are triggered by the oscillations of the magnet ring. Right: Representation of the mathematical domain.

The boundary conditions define the operating point of WMBP. For the fluid sub-problem, the hydraulic resistance in the pump, that is the head pressure H , is prescribed by means of a pair of Neumann conditions at the



inlet Γ^{in} and at the outlet Γ^{out} ; while non-slip wall conditions are imposed at boundary Γ^w :

$$\mathbf{T}^f(\mathbf{u}, p) \mathbf{n}^f = \mathbf{0} \quad \text{on } \Gamma^{in}, \quad (6)$$

$$\mathbf{T}^f(\mathbf{u}, p) \mathbf{n}^f = H \mathbf{n}^f \quad \text{on } \Gamma^{out}, \quad (7)$$

$$\mathbf{u} = \mathbf{0} \quad \text{on } \Gamma^w, \quad (8)$$

The progressive undulations in the membrane are caused by the oscillations of the magnet ring with boundary Γ_2^s ; then, they are transmitted to the external edge of the membrane Γ_1^s . Such oscillations are assumed to be purely sinusoidal with frequency f and amplitude Φ . Thus, the oscillations are prescribed by means of a Dirichlet condition on boundaries Γ_i^s ($i = 1, 2$):

$$\mathbf{d}(t) = \Phi \sin(2\pi f t) \mathbf{e}_z \quad \text{on } \Gamma^s \quad (9)$$

The benchmark consists in the validation of a numerical method to solve the FSI problem in WMBP against real hydraulic data provided by CorWave SA. Specifically, the goal is to predict the outflow volume rate Q^{sim} given a certain operating point of the pump (H, f, Φ) and compare the numerical result with the measured flow data Q^{data} .

In this report, we will describe the steps to take to solve the FSI problem with our numerical strategy, based on the Extended Finite Element Method (XFEM) [3, 4]. XFEM is an unfitted technique which has two main advantages compared with other approaches for FSI problems: i) since the fluid mesh is kept fixed on the background, it avoids the remeshing procedure normally occurring in case of element distortion; ii) the accuracy of the solution is maintained at the interface, thanks to the local enrichment of the functional space of the extended finite elements. However, since the structure mesh moves in the foreground cutting the underlying fluid mesh, XFEM requires to compute the mesh intersections at each time instant to identify the fluid elements that are cut in multiple subportions (called *split elements*), leading to a higher computational cost. For more details on the numerical formulation of the XFEM with a DG mortaring at the interface, the reader can find an exhaustive explanation in the reference papers [5, 6].

2. Input data

Input data to run the benchmark consist of four different types of files:

1. **meshes**: a folder that contains the fluid mesh, the membrane mesh and the magnet mesh;
2. **dataFile**: it details the list of meshes, physical parameters, stability parameters, operating parameters, time settings and other numerical parameters;
3. **solverFile**: it contains the parameters for the linear solver;
4. **validation data**: a csv datafile that collects the experimental data to be used to validate the numerical results

2.1. Meshes

For this benchmark, we consider the flat membrane pump geometry, studied in [5]. The CAD geometry files have been provided by the partner company CorWave SA. The unfitted meshes, reported in Figure 2, have been created using GMESH. The unfitted meshes selected for this benchmark showed positive convergence results. Lengths are expressed in *cm*.



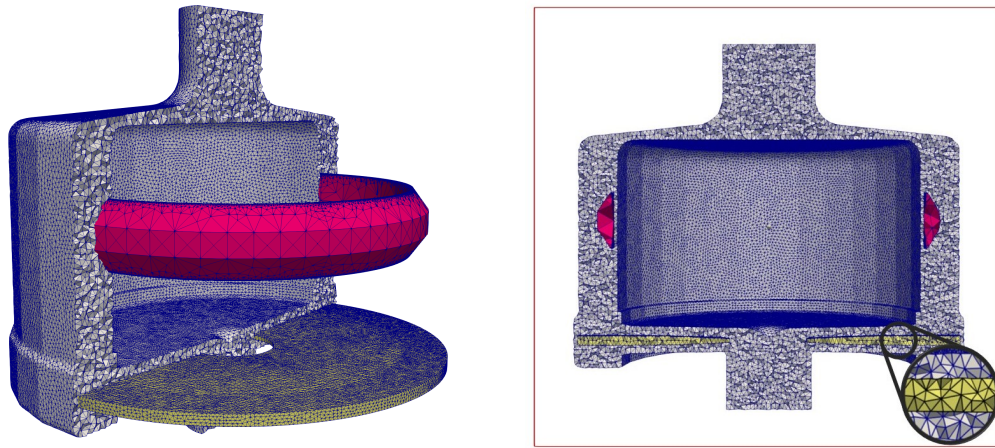


Figure 2: Prospective visualization and section of the fluid mesh (gray), the membrane mesh (yellow) and magnet mesh (red).

2.2. DataFile

The dataFile presents important information for the simulations, such as physical properties of the fluid and of the structures, discretization parameters, Operating Point (OP) parameters, Continuous Interior Penalty (CIP) stability parameters, and many others. The default values of all these data are reported in Table 1.

| Section | Variable | Value |
|--------------------------|--------------------------------------|--|
| Blood properties | Density ρ_f | $1 \frac{g}{cm^3}$ |
| | Viscosity μ_f | $0.035 \frac{dyne}{cm^2}$ |
| Membrane properties | Density ρ_s^1 | $1.125 \frac{g}{cm^3}$ |
| | Young Modulus E_s^1 | $1.686 \cdot 10^7 \frac{dyne}{cm^2}$ |
| | Poisson ration ν_s^1 | 0.49 |
| Magnet properties | Density ρ_s^2 | $7.85 \frac{g}{cm^3}$ |
| | Young Modulus E_s^2 | $2.05 \cdot 10^{12} \frac{dyne}{cm^2}$ |
| | Poisson ration ν_s^2 | 0.28 |
| OP parameters | Head Pressure H (*) | 50 mmHg |
| | Frequency f | 120 Hz |
| | Amplitude Φ | 0.053 mm |
| Stability CIP parameters | Convection control γ_{v1} (*) | 0.05 |
| | Divergence control γ_{v2} (*) | 0.5 |
| | Inf-sup control γ_p (*) | 0.05 |
| Time settings | Initial time t_0 | 0 s |
| | Final time T | 0.025 s |
| | Time step Δt | 0.0002 s |

Table 1: Default physical and discretization parameters defined in dataFile. Variables with (*) can be modified.

The experimental data for the validation are provided only for oscillation frequency of 120 Hz and amplitude Φ of 0.053 cm. Hence they should not be changed. Also notice that pressure conditions can largely affect the pump dynamics and consequently the stability requirements. For this reason, we suggest the user to set the head pressure parameter H and the CIP penalty parameters according to Table 2. All parameters are expressed in the unit system *cgs*.



| | $H = 50$ mmHg | $H = 55$ mmHg | $H = 60$ mmHg |
|---------------|---------------|---------------|---------------|
| γ_{v1} | 0.05 | 0.05 | 0.5 |
| γ_{v2} | 0.5 | 0.5 | 5 |
| γ_p | 0.05 | 0.1 | 0.1 |

Table 2: Continuous Interior Penalty parameters for different head pressure conditions.

Additional information in the DataFile include the strings of the mesh files (fluid: 1.2M elements, membrane: 300k elements, magnet: 50k elements) and of the solverFile (solverFile.xml is the default) and other preconditioner settings.

2.3. SolverFile

The solverFile, reported in Appendix A.1, collects some numerical settings for the solver of the linear system. In general, such parameters should be kept fixed for parallel runs with more than 3 processors (10 cores are suggested to reduce computational cost). In case of serial runs or less than 3 processors, the user has to reduce the dimension of Krylov space (kspace) to 200 and of the number of maximum iterations (max_iter) to 500. Hence, in this case use file *SolverFile_serial.xml*.

2.4. Validation data

The experimental data used for the benchmark are *HQ curves* (H head pressure, Q flow rate), which are standard representations of pump hydraulic performance. They are obtained during the *in vitro* testings in a pump characterization bench, measuring the pressure difference H between the outlet and the inlet (called head pressure), and the corresponding flow rate Q generated at the outlet. The head pressure represents the hydraulic resistance of the system (adverse pressure gradient), that has to be overcome to generate pump outflow. Figure 3 shows the HQ curve of the pump system when the frequency of oscillation of the membrane is fixed to 120 Hz and the amplitude of oscillation to 0.053 cm. Notice that the flow rate decreases as the head pressure increases, owing to the higher hydraulic resistance in the pump. Raw data are provided in the Excel file *HQ_curve.csv*, consisting of two separate data columns with the measurements of head pressure in mmHg (1 mmHg = 1333.22 g/cm²) and of the outflow volume rate in liters per minute, or lpm (1 lpm = 0.06 cm³/s).

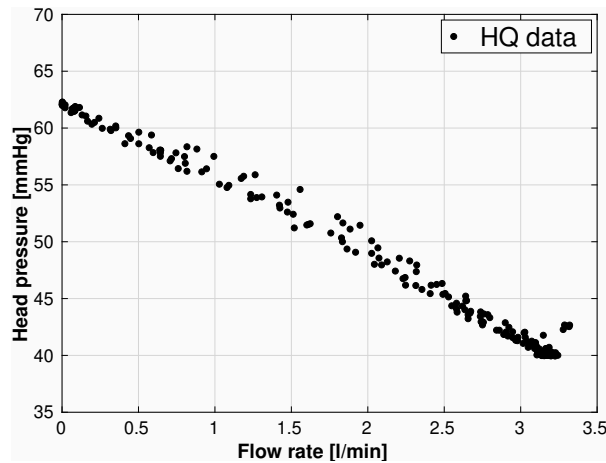


Figure 3: HQ experimental curve at oscillation frequency $f = 120$ Hz and amplitude $\Phi = 0.053$ cm.



3. Output data

The output of interest for this benchmark is the flow volume rate at the pump outlet Γ^{out} . Indeed, the goal is to compare, for a certain input head pressure H , the corresponding estimated outflow rate Q^{sim} with the experimental data Q^{data} extracted from the HQ curves (see Figure 3). At each time iteration, the software prints out the outflow computed at that time instant. Since this quantity oscillates in time with frequency f , we need to compute the average in time of the outflow results at regime, i.e. during the last period of oscillation τ . Thus:

$$Q^{sim} = \int_{T-\tau}^T \int_{\Gamma^{out}} \mathbf{u}(\mathbf{x}, t) \cdot \mathbf{n} d\mathbf{x} dt \quad (10)$$

Finally, a Python script can be used to plot the HQ curve and the obtained numerical results Q^{sim} to check their proximity and compute absolute and relative errors. The user has just to type in the simulated head pressure H . In Table 3 we show the expected results for this benchmark for certain head pressure conditions, as reported in [5].

| | $\Delta P = 50 \text{ mmHg}$ | $\Delta P = 55 \text{ mmHg}$ | $\Delta P = 60 \text{ mmHg}$ |
|------------------------|------------------------------|------------------------------|------------------------------|
| Q^{data} | $1.834 \frac{1}{\text{min}}$ | $1.091 \frac{1}{\text{min}}$ | $0.352 \frac{1}{\text{min}}$ |
| Q^{sim} | $1.792 \frac{1}{\text{min}}$ | $1.039 \frac{1}{\text{min}}$ | $0.400 \frac{1}{\text{min}}$ |
| $ Q^{data} - Q^{sim} $ | $0.042 \frac{1}{\text{min}}$ | $0.052 \frac{1}{\text{min}}$ | $0.048 \frac{1}{\text{min}}$ |

Table 3: Experimental and simulation data for the model validation against experimental mesures.

4. Procedure

The aim of the proposed benchmark is to validate the FSI model via comparison of the numerical results against experimental HQ curves in wave membrane blood pumps. In this section, we explain the steps to take to install the software, set the data, run the FSI simulations and post-process the computed numerical results.

4.1. Step 0: Installation

The material to run the benchmark, including source files, validation data and post-processing tool, is available in the GitHub repository at <https://github.com/ROMSOC/validation-wmbp> and can be downloaded or clone in your local machine. In addition, a DockerFile is provided to generate an Ubuntu image with the LifeV environment and all the additional libraries required to solve this benchmark. The user can use the DockerFile to build the Docker image with a certain TAG (e.g. martin592/validation-wmbp:env)

```
docker build -f DockerFile -t [TAG] .
```

or pull the corresponding public image from DockerHub (free registration to <https://hub.docker.com/> is required). In this case, it is sufficient to type:

```
docker pull martin592/validation-wmbp:env
```

Finally a Docker container can be generated using file runLifeV.sh:

```
./runLifeV.sh
```

Now you should have created a Docker LifeV container, including a copy of all the folders in the benchmark repository and all the libraries required to run the benchmark. In addition, all the changes in the container will be copied in the local repository.



4.2. Step 1: Setting input data

Move to the benchmark/ subfolder. The input data needed to run the simulations include i) the meshes/ folder, ii) the dataFile, and iii) the solverFile. Check that all these documents are present in the working directory.

Most of the input settings need to be maintained fixed for this benchmark. However, the user should set the head pressure H (in mmHg) in the pump by changing variable [OP/pressure] in the dataFile (default value is 50 mmHg). We suggest also to change the penalty parameters at lines [penalty] of the dataFile, according to what indicated in Table 2 to ensure stability.

Finally, in case of serial runs or for parallel runs with less than 4 processors, change the variable [prec/paramListFile] to solverFile_serial.txt. Also, move solverFile_serial.txt from paramsFile/ subfolder into the working directory.

4.3. Step 2: Run simulations

To run the FSI simulations in wave membrane blood pumps, it is sufficient to execute the program with the following command from command line:

```
./WMBP.exe -f dataFile > benchmark_output.txt
```

in case of serial runs, or

```
mpirun -np 7 WMBP.exe -f dataFile > benchmark_output.txt
```

in case of parallel runs with a number of processors equal to 7.

Notice that these simulations can last for several days and require a minimum of 40 GB of RAM for serial runs. In addition, simulation may stop due to the failure of external library tetgen, trying to solve particularly complex geometric sub-problems, inherent to XFEM-based strategy. In this case, the user should restart the simulation from the last saved time step, following the instructions detailed in the Appendix A.2.

4.4. Step 3: Post-processing

The numerical results of interest for this benchmark consist of the flow rate at the outlet. At each time instant, the software prints the computed outflow rate in the output file benchmark_output.txt. Hence, move to post-processing/ sub-directory and copy the output file benchmark_output.txt in it.

Post-processing is structured in two steps:

1. extract the time series of the outflow rate from the output file benchmark_output.txt using Python script extract_flowResults.py as follows:

```
python extract_flowResults.py benchmark_output.txt .
```

2. run the Python code validation.py

```
python validation.py
```

to compute the mean flow rate Q^{sim} as in Equation 10, plot it with the HQ data curve, and compute the numerical error.

A Python installation (version ≥ 2.7) is required, together with Python packages numpy and matplotlib.

References

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- [3] E. Burman and M. A. Fernández, “An unfitted Nitsche method for incompressible fluid–structure interaction using overlapping meshes,” *Computer Methods in Applied Mechanics and Engineering*, vol. 279, pp. 497–514, 2014.
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- [6] S. Zonca, C. Vergara, and L. Formaggia, “An unfitted formulation for the interaction of an incompressible fluid with a thick structure via an XFEM/DG approach,” *SIAM Journal on Scientific Computing*, vol. 40, no. 1, pp. B59–B84, 2018.



A. Appendix

A.1. SolverFile.xml

Listing 1: solverFile.xml

```
<ParameterList>
<!-- LinearSolver parameters -->
<Parameter name="Reuse Preconditioner" type="bool" value="false"/>
<Parameter name="Max Iterations For Reuse" type="int" value="80"/>
<Parameter name="Quit On Failure" type="bool" value="false"/>
<Parameter name="Silent" type="bool" value="false"/>
<Parameter name="Solver Type" type="string" value="Aztec00"/>

<!-- Operator specific parameters (Aztec00) -->
<ParameterList name="Solver: Operator List">

<!-- Trilinos parameters -->
<ParameterList name="Trilinos: Aztec00 List">
<Parameter name="solver" type="string" value="gmres"/>
<Parameter name="conv" type="string" value="rhs"/>
<Parameter name="scaling" type="string" value="none"/>
<Parameter name="output" type="string" value="all"/>
<Parameter name="tol" type="double" value="1.e-6"/>
<Parameter name="max_iter" type="int" value="4000"/>
<Parameter name="kspace" type="int" value="2000"/>
<!-- az_aztec_defs.h -->
<!-- #define AZ_classic 0 /* Does double classic */ -->
<Parameter name="orthog" type="int" value="0"/>
<!-- az_aztec_defs.h -->
<!-- #define AZ_resid 0 -->
<Parameter name="aux_vec" type="int" value="0"/>
</ParameterList>
</ParameterList>
</ParameterList>
```

A.2. Simulation - Restart

In case of running error, a restart procedure has to be carried over to continue the simulation from the last saved timestep. At each time instant, the software exports the fluid and solid solutions in .h5 and .xmf format, that can be used to restart the job. For instance, at time iteration 39, the exported restart files are: fsiRestartF_039 (fluid), fsiRestartS1_039 (membrane) and fsiRestartS2_039 (magnet).

The restart procedure consists of two steps:

1. Define the settings of dataFile_restart as in dataFile. In addition, the user has to specify:
 - i) the restart time iteration [importer/initTimeIter] (e.g. to 39), and ii) the corresponding initial time [time_discretization/initialtime] (in s).
2. restart the simulation by typing on the command line:

```
mpirun -np 7 WMBP.exe -f dataFile_restart > benchmark_output_restart.txt
```

This can be run either in serial or in parallel, as in Section 4.3. Check that the restart files are present in the working directory for both the restart time iteration AND the previous one, e.g. fsiRestart*_039



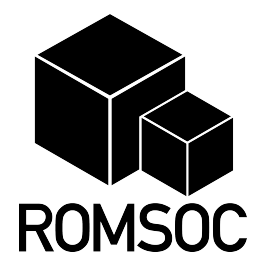
and `fsiRestart*_038`.

Notice that for the post-processing of a simulation that required a restart, the results need to be extracted also from output file `benchmark_output_restart.txt`. Hence, the user has to run:

```
python extract_flowResults.py benchmark_output_restart.txt
```

and join the results together in a unique file `flowResults.txt`.





The ROMSOC project

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