Comparison of one- and two-way coupling of Fluid-Structure Interaction model of peristaltic pump

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Abstract: Peristaltic pumps are used during pharmaceutical manufacturing processes, for several unit operations. Goal of this work was to develop a computational model of a peristaltic pump used for filling operations, to predict shear stresses and mass flow rates. For this purpose, COMSOL software was used to create a multi-physics model of a peristaltic pump, an elastomeric tube and a viscous Newtonian fluid.

The tube deformation is modeled using the Nonlinear Structural Materials Module, assuming Hyperelastic properties. The fluid is modeled using the CFD module, assuming Laminar flow. In summary, it is a Fluid-Structure Interaction (FSI) problem that can be solved either with one-way coupling (first solid, then fluid part) or two-way coupling (full FSI). The two approaches are compared in terms of differences in predicted values and computational cost.

Simulations are all performed on Rescale Cloud Computing platform using COMSOL Server™. Prerequisite for that is the creation of an application of the model. The model is created in a local workstation with a CPU license and converted into an app using the Application Builder tool. The app is then uploaded on Rescale platform to perform the simulation. After successful completion of simulation, the app is saved and downloaded locally for further analysis and post-processing.

Keywords: Fluid-Structure interaction, Peristaltic pump, Hyperelastic modeling, COMSOL Server, Simulation app

1. Introduction

Peristaltic pumps find applications in pharmaceutical, chemical and food industries. Specifically, for pharmaceutical manufacturing processes, peristaltic pumps are the preferred option, used in filling, filtration and mixing operations. Additionally, current setups for implementation of online measurement tools rely on peristaltic pumps to form an external loop allowing for plug-and-play integration of sensors and Process Analytical Technology (PAT) tools.

Peristaltic pumps are a type of positive displacement pumps, where a tube is squeezed by a set of rollers causing the fluid inside it to move. In recent years, there were several publications from the pharmaceutical industry investigating peristaltic pumps experimentally, mainly related to particle shedding and particle formation in biologic drug products [1]–[5]. However, there are only a few available numerical studies of peristaltic pumps in open literature [5]–[9]. One of the first actual fluid-structure interaction models of a peristaltic pump was presented by Elabbasi et al. [6], also created on COMSOL Multiphysics. Goal of this work was to create a model of a peristaltic pump that is employed during fill & finish operations of a biopharmaceutical drug product which can be used to predict shear stresses on the fluid. The model development and results of this work are discussed in the following chapters.

2. Computational methodology

A model of a peristatlic pump, that is used for filling operations of biologic drug products in glass containers, has been created in COMSOL. It is an inherently multiphysics problem where the deformation of the tube and the pumped fluid are strongly coupled. The model of the pump is presented in Figure 1.

It consists of a housing, a set of rollers and an elastomeric tube, pumping a viscous Newtonian fluid.

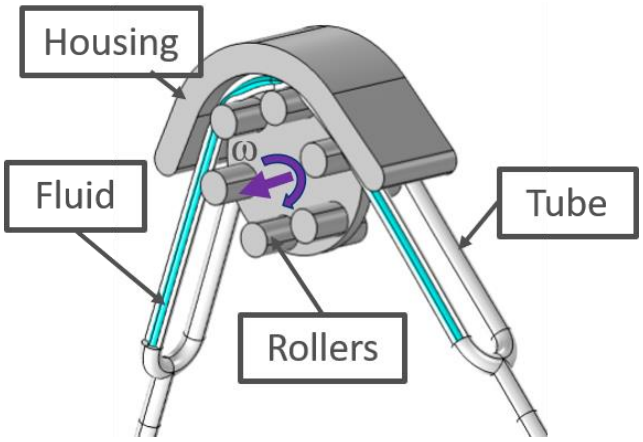

Figure 1: Model of a peristaltic pump created in COMSOL Multiphysics

Depending on the number of rollers and configuration of the pump, it is well known that peristaltic pumps may induce oscillations on the flow rate, consistent with the engaging and disengaging of the rollers on the tube. For filling operations, filling accuracy is of paramount importance. For this reason, these devices typically have two sets of rollers, positioned at a different angle. An elastomeric tube is squeezed between each set of rollers and the housing. The two tubes are connected at inlet and outlet with additional tubes through Y-pieces. In that way, the flow streams of each tube are connected in one and the mass flow oscillations of each stream counter-balance each other, leading to a more steady flow at outlet. The modeled device has two sets of six rollers, positioned at an angle of 30° relatively to each other.

Due to the complex, asymmetrical design of the housing and set of rollers, it is not possible to have a prescribed shape of the elastomeric tube. For this reason, the simulation strategy of this model was split in two parts and is presented in Figure 2. In the initial model configuration, the rollers are out-of-position and the elastomeric tube is straight and unstressed between the rotor and the housing. The rotor is then displaced to its correct position in a transient simulation until the tube is squeezed between the rollers and the housing. That way it is possible to acquire the initial pump configuration and the natural deformation and stress levels of the elastomeric tube.

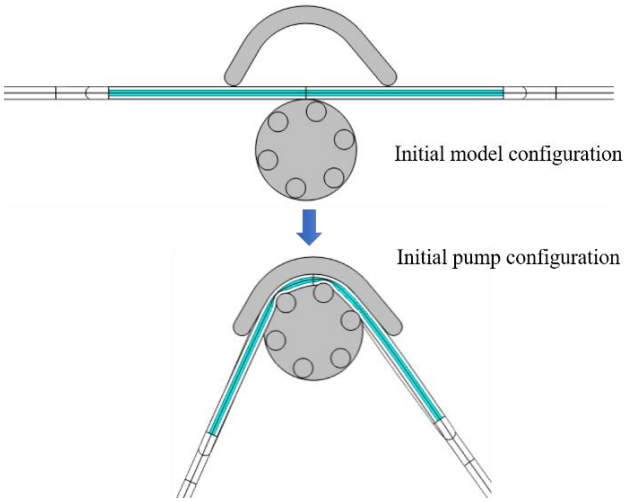

Figure 2: Rollers are displaced to get the correct pump configuration

The next step is to run a transient simulation modeling the rotation of the rotor and the flow that is induced as a result. This is modeled with a prescribed rotation of the rotor. It is a strongly coupled Fluid-Structure Interaction (FSI) problem and it can be approached with two different methods, as shown in Figure 3. The first method is the one-way coupling, where the solid mechanics is solved first, i.e. rotation of the rotor and tube deformation over time. It is then followed by the fluid dynamics problem, which uses the solution of the solid mechanics for the unsolved variables. The second approach is to solve both solid and fluid fields simultaneously.

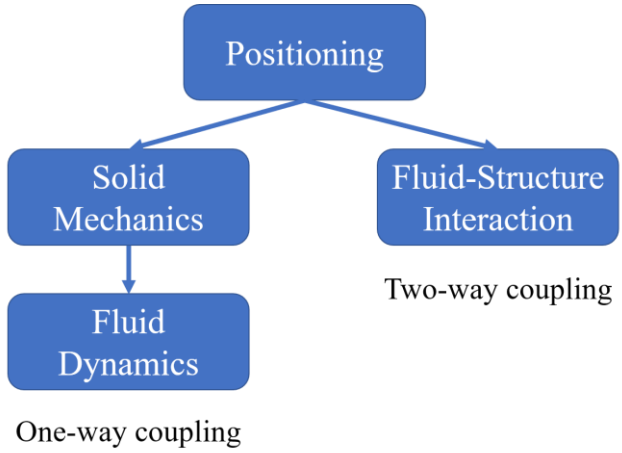

Figure 3: One- and two-way coupling approach for the simulation

In general, it is considered that the two-way coupling approach leads to more accurate predictions, but it is very case-dependent and there is not enough data available in open literature. Both methods have advantages and disadvantages in terms of computational cost, memory requirements and solution accuracy. One of the goals of this work was to investigate the different approaches further and to present preliminary results.

2.1 Model setup

The tubes that are used in peristaltic pumps are typically made of elastomeric material such as silicone or thermoplastic elastomers. The tube is modeled assuming a hyperelastic material with a standard Mooney-Rivlin material model. The tube material properties that were used are typical values of elastomeric material but for higher accuracy of the solid mechanics predictions it is recommended to characterize these values experimentally.

The housing of the pump, as well as the rotor and rollers, are defined in the model as separate rigid domains. This assumption is feasible, considering that these bodies are much stiffer compared to the elastomeric tube and there is negligible deformation, if any at all. The degrees of freedom are also reduced in that way, reducing the required simulation time. Several contact pairs are defined between the tube and rollers and housing, with the tube surfaces always defined as a “destination” boundary, due to significantly lower stiffness. The penalty formulation was used for the contact method. Alternatively, the Augmented Lagrangian formulation can be used, which leads in general to more accurate modeling of the contact surfaces. However, it has higher computational cost and poses limitations on the solver that can be used, as it can only be solved using a segregated solver. Finally, frictionless contact is assumed between the surfaces. In reality the rollers are free to rotate, leading to rolling contact and lower friction forces than sliding contact. Rotating rollers could be implemented with the Multibody Dynamics COMSOL module, but this was out of scope of this study.

The fluid flow inside the tube is described by the Navier-Stokes equation, assuming laminar and incompressible flow of a Newtonian fluid with water-like properties. The boundaries at inlet and outlet of the domain are assigned as open boundaries.

For the fluid-structure interaction problem, COMSOL automatically assigns a no-slip boundary at the inner wall of the tube and uses an Arbitrary Lagrangian-Eulerian (ALE) formulation. As the tube is deformed with the roller rotation, the fluid domain and its mesh should also be deformed accordingly. This was resolved with a moving mesh model with a hyperelastic mesh smoothing type. The difference between one- and two-way coupling approach is the information transferred between the solid and fluid domain. For one-way coupling, only the wall velocity is transferred to the fluid and there is no impact from the fluid forces on the tube deformation. On the other hand, for the fully coupled case, the fluid loading on the structure is also taken into account.

Finally, the positioning, as well as the solid and fluid simulations of the first approach are solved with a segregated, direct solver. However, for the fully coupled FSI it was not

possible to start the simulation with a segregated solver. Only a fully coupled solver worked for this case, probably due to the highly nonlinear nature of the problem.

2.2 Simulation app and COMSOL Server

As presented in the previous chapter, the model of this peristaltic pump is rather complex, consisting of many different parts and offering no chance to utilize a symmetry plane, due to the asymmetrical design of the setup. As a result, the mesh requirements and computational cost increased dramatically.

In the beginning of this study, some simulations of the one-way coupling approach were performed on a local workstation, but the available computational resources posed a significant bottleneck on the completion of the project. The simulation wall time was more than one week and only one simulation could be performed at a time, due to low number of cores and available RAM memory.

All internal COMSOL simulations were migrated to a High-Performance Computing (HPC) platform to reduce computational time of each simulation. The platform of choice was Rescale, as it was already established internally for other computational applications. Rescale is a cloud computing platform that offers several different types of hardware and is used on-demand. A user can select one of the available hardware configurations, as well as the number of cores that need to be allocated. The different hardware configurations are named after minerals or precious stones, such Onyx or Ruby. After several tests, it was concluded that the Emerald configuration is the optimum solution for COMSOL simulations and was selected for conducting this study. The technical specifications of the local workstation, as well as of Rescale's Emerald configuration, are presented in Table 1.

Table 1: Technical specifications of available platforms.

Platform	CPU type	RAM	Nr of cores
Local workstation	Intel Xeon E5-2623 v3 @ 3.0 GHz	32 GB	4
Rescale - Emerald	Intel Xeon Platinum P-8124 (Skylake) @ 3.0 GHz	144 GB (4GB/core)	36

In combination with Rescale HPC cloud platform, COMSOL Server was used for the performance of this study. COMSOL Server allows the user to run simultaneously up to four simulations per license package. This can speed up base business considerably compared to running simulations serially in the existing local workstation. In order to use COMSOL Server, the model needs to be converted into an application file. This can be performed after model development in the local workstation using a typical CPU license. Then, the app is uploaded on the cloud platform and the simulation runs utilizing the HPC resources. Finally, the file is downloaded again locally for further post-processing and analysis of the results.

Comparison of computational times and memory requirements, as well as results of the simulations are presented in the following chapter.

3. Results and discussion

3.1 Computational time and memory requirements

At the beginning of using Rescale platform, several tests were conducted to assess strong scaling. Strong scaling concerns the speedup for a fixed problem size with respect to the number of processors, and is governed by Amdahl's law [10]. Data from Rescale's Emerald configuration for different number of cores are compared with the performance of the local workstation.

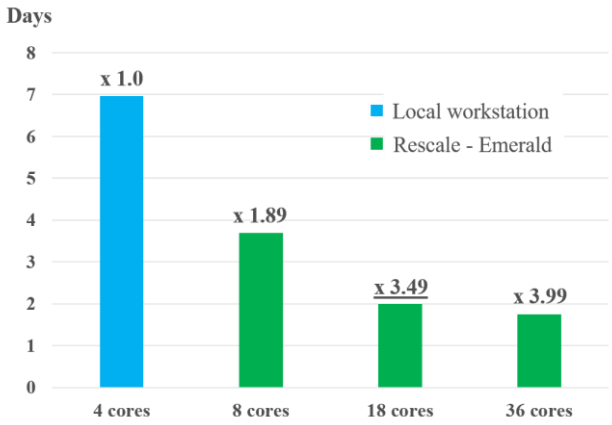

Figure 4: Computational cost for different multicore configurations

The test case that was used was the one-way coupling approach of the presented model. The simulation included the positioning step, as well as the solid and fluid simulation for two complete rotor revolutions. The reason for this choice was that internal tests and previous references have shown that for many pump configurations the initial transients die out after at least one rotor revolution [6]. As presented in Figure 4, the simulation required seven days to finish in the local workstation. The exact same test case was simulated on Rescale using Emerald configuration, allocating 8-, 18-, and 36-cores. As seen in the graph, there is considerable speedup when using the HPC resources for all cases. More specifically, the simulation was completed in less than two days when at least 18 cores were allocated, achieving a speedup by a factor of x3.5. It is very interesting, however, to notice that the speedup from 18 to 36 cores is relatively small, while the cost of resource allocations is doubled. Depending on the model size, using 36 cores could actually be slower than using 18 cores. This can be explained considering that the communication overhead between cores increases and the speedup offered by splitting the problem in more cores may not be enough to compensate, resulting in a slowdown of the simulation. This means that it is not always advised to use the maximum number of available cores. Often, delivery times and cost should be considered when choosing the number of cores and should be backed up by appropriate scaling tests.

The improvement that can be achieved using COMSOL Server with the HPC platform is considerable and can be illustrated with the following example. Assuming a request was received

to run the pump model with four different setups (i.e. different RMP or tube dimensions), it would require 28 (4x7) days of just pure computational time to perform in the local workstation. This can be reduced to just 2 days by running all cases simultaneously on the much faster hardware of the cloud platform, achieving a massive speedup by a factor of x14.

After these tests, the two-way coupling was also submitted for simulation on Rescale. The simulation was again intended to complete two rotor revolutions. Unfortunately, the simulation crashed after completing almost 85% of the first revolution. Although the reason has not been fully defined, there are some indication that will be discussed in the following chapter.

A fully coupled solver was used for the two-way coupling approach, as it was not possible to even start the simulation with a segregated solver. This posed a new challenge in performing the simulation which was related to available RAM memory. The total degrees of freedom as reported in COMSOL log output file were more than 2.4 million. This required about 37 GB and 130 GB of RAM when the iterative and direct solver were used, respectively. Both requirements exceeded the available memory on the local workstation, so it was not possible to perform this simulation on the local workstation or on Rescale with fewer than 36 cores. The estimated time for completion of two rotor revolutions was 12 days when using a fully coupled, iterative solver. This is about 6 times slower compared to the one-way coupling approach.

3.2 Simulation outputs

One purpose of the developed model is to predict shear rates in the fluid domain. Biologic drug products, such as monoclonal antibodies, are sensitive to shear, which can lead to protein unfolding or particle formation and thus reducing the efficacy of the drug product. Such an effect on the product must be avoided under all circumstances. Since it is very difficult to measure shear rates directly during the experiment, it is important to develop a model to predict developed stresses.

Figure 5 shows the predicted stresses on the tube, as well as the velocity contours of the fluid inside the tube for one timestep, at 65% of the rotor revolution. The pump speed was 350 RPM, which is the target speed of this pump for filling operations. It is clearly shown that the maximum stresses on the tube are close to the regions in contact with the rollers, where the change of curvature of the tube is maximum.

It is also seen that the tube occlusion is not uniform between the three rollers that are in contact, due to the asymmetric design of the housing. The minimum gap at all timesteps is less than 0.2mm. It is important to mention that in many applications, the rollers cause full occlusion of the tube. However, such a case is not possible to describe numerically. If the inner surfaces of the tube come in contact, the mesh points of the fluid domain will locally collapse, creating singularities and the solver is not able to handle this. Therefore, this type of model can provide a worst-case scenario, where the predicted values of shear rate close to maximum occlusion may be larger than those developed in reality during operation.

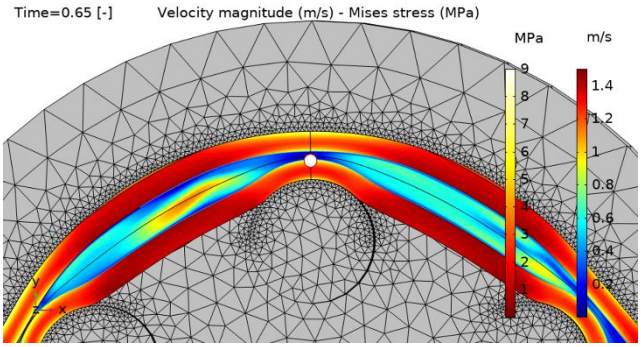

Figure 5: Tube stress and velocity contours

In order to analyze further, the time-dependent results of a single point on the fluid-structure interface are presented in Figure 6. The point can be seen as a white dot in the inner surface of the tube, above the middle roller, in Figure 5. As seen in Figure 6a, the Mises stress of the tube at that point shows a nicely periodic behavior over time, consistent with the rotor rotation. Also, there is no difference observed between the two approaches. It is important to mention that this behavior is related to the fact that the fluid has low viscosity (1 cP). This could change if the viscous fluid forces are higher due to high fluid viscosity.

However, the situation is different looking at the predicted shear rate in Figure 6b. Both in one- and two-way coupling, there appear to be high frequency oscillations. A similar pattern was identified at total inlet and outlet flow rates. This behavior cannot be explained physically and could be related to the crash of the two-way coupling simulation. The reason behind it has not been fully identified at the current stage of this work and additional tests are required to investigate. As observed in Figure 6c and d, the mesh displacement of this point in x and z coordinate also show large variations over time. These oscillations are transferred to the wall velocity and the impact can be seen in the shear rate and flow rate values.

There are several measures to investigate further and resolve this numerical problem. The first one is a mesh- and timestep sensitivity analysis. Additionally, some damping properties may be introduced to the hyperelastic material, as currently, no damping was used for this study. Finally, as mentioned previously, frictionless contact is assumed for all surfaces. The introduction of a small friction coefficient could help dampen these high frequency oscillations. All these measures could help improve the numerical stability of the simulation overall and will be the focus of future work.

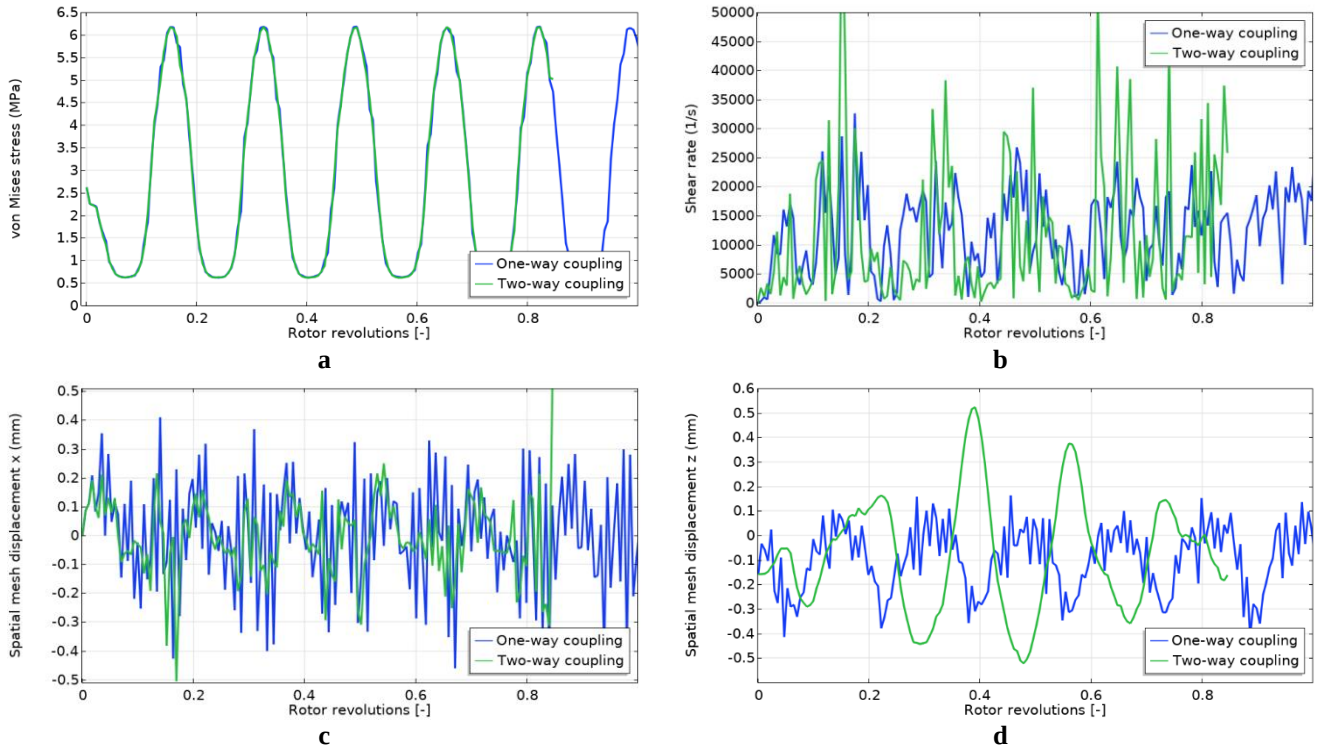

Figure 6: Time-dependent parameters for a single point on the fluid-structure interface – a) von Mises stress, b) Shear rate, c & d) Spatial mesh displacement in x and z direction

4. Conclusions

A computational model of a peristaltic pump, that is typically used for filling operations of biologic drug products, has been created using COMSOL Multiphysics. In order to accelerate the numerical simulations, it was decided to migrate them from a local workstation to a high-performance cloud computing platform. The model was created locally, converted into an application and was then simulated on the cloud platform using COMSOL Server.

Through initial strong scaling tests, it was demonstrated that for the cases under investigation, a speedup by a factor of almost 4 is achievable by switching to cloud computing. It was also shown that the gained speed does not increase linearly with the number of allocated cores. Delivery times and cost should be considered when choosing the allocated cores number. Finally, COMSOL server offers the capability to run four applications simultaneously, which decreases the required simulation time of a hypothetical base business case from 28 days to just 2 days. This is a considerable improvement and will add a lot of value to the current computational capabilities.

The fluid-structure interaction problem was solved with two different approaches; sequentially and fully coupled. It was shown that the fully coupled method is much more demanding in terms of computational resources, requiring six times more computational time to completion and almost four times higher RAM memory.

Unfortunately, due to the highly nonlinear nature of the problem, the simulations were numerically unstable at the current stage of this work, not allowing a direct comparison of the results and the differences of the two methods.

Nevertheless, the presented work explains the methodology on creating and running such a model and sets a solid foundation for further investigations.

5. Acknowledgements

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6. Abbreviations

ALE	Arbitrary Lagrangian-Eulerian
CPU	Central Processing Unit
FSI	Fluid-Structure Interaction
HPC	High-Performance Computing
PAT	Process Analytical Technology
RPM	Revolutions Per Minute

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