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SCALABILITY STUDY OF THE PARALLEL PARTITIONED MULTI-PHYSICS SIMULATION FRAMEWORK

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Abstract. Fluid Structure Interaction (FSI) is a multi-physics problem that dominates many engineering and research applications. In this work we present a partitioned FSI framework developed around a number of open-source solvers and an open-source general purpose code coupling library. Fluid dynamics are handled by OpenFOAM and a solid mechanics solution is implemented in FEniCS. A scalable and portable coupling is achieved via the Multiscale Universal Interface (MUI) library that builds an interface between the coupled codes using MPI, with the potential to scale to hundreds of thousand of MPI ranks. The validity and the performance of the framework will be tested via a series of FSI benchmark cases using the UK's national supercomputing service ARCHER2.

1 INTRODUCTION

Fluid structure Interaction (FSI) is a multi-physics problem in which fluid dynamics is influenced by the kinematics of structural components and vice versa. It dominates a wide range of engineering and research applications, ranging from large-scale problems such as floating wind farms and wind turbine blades through to much smaller scales such as blood flow in arteries. Studying FSI is challenging due to the involvement of nonlinear behaviours at different temporal and spatial scales. Laboratory experiments are typically limited in defining the full dynamics of an FSI problem, while numerical simulations can provide a comprehensive insight into a complete solution. However, robust and accurate numerical simulation of FSI is often computationally expensive and can involve billions of degrees of freedom [1]. Works to develop an FSI framework capable of scaling to current petascale and even future exascale levels of computing are limited, even more so when work involving only open-source solutions are considered.

In this work we present a study into the accuracy and the performance of an in-house open-source multiphase FSI framework called the Parallel Partitioned Multi-physics Simulation Framework (ParaSiF) [1] [2, 3]. The framework is designed as wholly partitioned; therefore different solvers are used for the fluid and structural parts of the problem, each run simultaneously but independently from the other. This allows for the separation of concerns in terms of the development of the FSI algorithm and also the implementation of each solver and permits the use of well established legacy codes to solve each component of the problem. Here the

[1] https://github.com/ParaSiF/ParaSiF

open-source codes OpenFOAM and FEniCS are used to solve the fluid and structure dynamic equations, respectively. A coupling interface between the fluid and structural domains has to be explicitly defined, and for this the MUI (Multiscale Universal Interface) coupling library is used to exchange data using only MPI [4, 5].

2 MULTIPHASE FSI FRAMEWORK

The presented framework can be used to study both single-phase and multiphase FSI problems by employing different OpenFOAM solvers. Figure 2 shows the algorithmic workflow of ParaSiF with the fluid dynamics solver on the left hand side of the flowchart, the structural mechanics solver on the right and a communication interface between the two. In the tests to be presented here, the fluid solution is provided by the *interFoam* which is an OpenFOAM application that solves the incompressible Navier–Stokes equations for two phases using the finite volume approach. The free surface between water and air is captured using the Volume of Fluid (VoF) method. Mesh movement is handled by the in-built capability within OpenFOAM using an approach similar to the Arbitrary Lagrangian Eulerian (ALE) method. Structural mechanics are approximated using a generalised n-DoF (degrees of freedom) harmonic oscillator equation. These are discretised using the finite-element method and the solution implemented in the general purpose FEniCS framework, specific implementation details can be found in [2, 3].

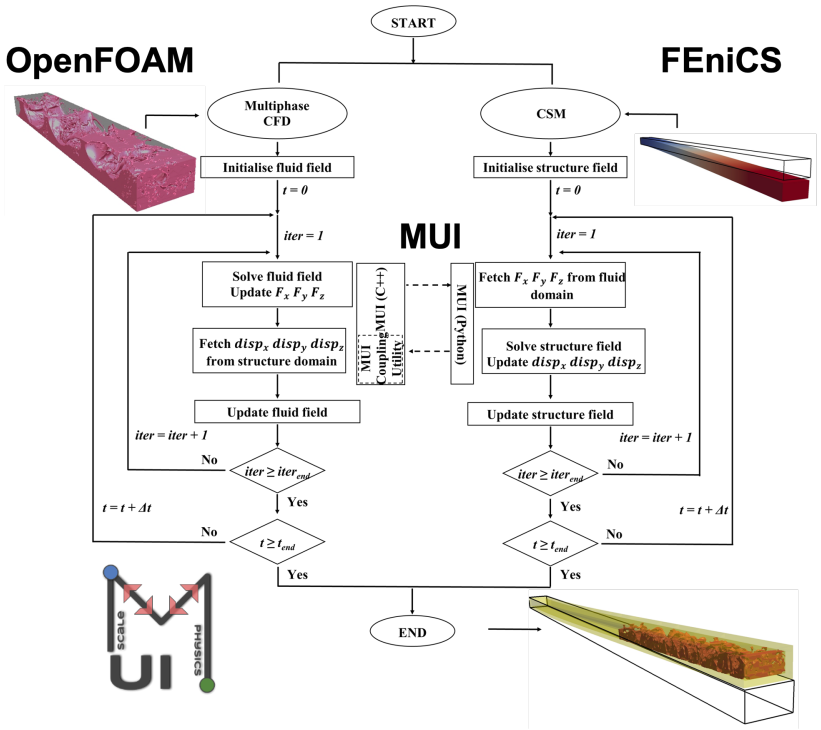

Figure 1: Diagram showing algorithmic design of ParaSiF [2].

The coupling library MUI is used to create the communication interface between the two solvers, this is an open-source C++ library (wrappers available for Fortran, C and Python) and is designed using purely MPI for data transport. The key advantages of MUI are i) minimal

changes are required to the existing code due to the adoption of a header only library approach, ii) MUI can universally handle different types of data structures thanks to the use of templates, and iii) it spatially represents data as a cloud of points on which it can perform temporal and spatial interpolation, this makes coupling between different discretisations or couplings involving a volumetric (overlapping) region relatively trivial to implement. In the case of ParaSiF temporal interpolation is not needed while a nearest neighbour spatial interpolation is used on the consistent of deformation and a Radial Basis Function (RBF) interpolation is employed ensuring the conservative of integrated forces at the coupling interface.

2.1 SCALABILITY TESTING

The scalability of ParaSiF on HPC facilities is dictated by how well each component of the solution performs as well as how the coupling interface itself scales. Both OpenFOAM and FEniCS are known to have good potential parallel performance and scale well up to thousands of cores [6, 7]. In Skillen *et al.*[8], it was shown that MUI is capable of good parallel performance up to $O(10^4)$ of MPI tasks. Combining these codes together, Liu *et al.* [9] conducted a scalability test by varying the number of MPI tasks in both the structure domain and the fluid domain, and showed a good performance with up to 500 and 1000 MPI tasks respectively, in this study we look at the scalability of the framework given recent developments around performance and use of the new UK's national supercomputing service, ARCHER2. In order to explore the potential parallel ability of MUI a stand-alone benchmark test case with a worst-case volumetric coupling in which all cells from one domain are transferred to the other has been run. The benchmark consists of two coupled domains of 500 million cells each with equal load-balancing and was conducted on ARCHER2. The results show that, without additional interpolation, MUI speed up is near ideal up to 50000 MPI tasks, application within ParaSiF will result in a significantly smaller communication overhead. Therefore the expectation is that scalability will be bound by the solvers. To explore the limits of this, a series of FSI benchmark cases will be used to investigate the performance and the scalability of the ParaSiF and the results presented.

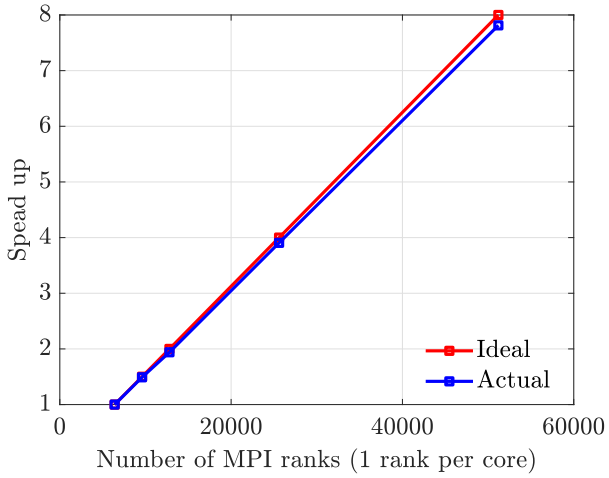

Figure 2: The parallel speed up performance of MUI communications

3 CONCLUSIONS

An in-house and open-source FSI framework named ParaSiF based on a fully partitioned approach is presented and its scaling on the ARCHER2 supercomputing service explored. ParaSiF is designed around well established legacy codes that are known to scale reasonably, OpenFOAM, FEniCS and then uses the open-source code coupling library MUI to connect them. This allows for a general-purpose FSI framework that is portable and flexible. Because it uses a fully partitioned approach, it presents opportunity to replace one solver with another (for example to achieve better scaling) or to introduce extra physics capability by coupling in extra solvers in the future.

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