An Innovative Partitioning Technology for Coupled Software Modules

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Abstract: Multi-physics simulation approaches by coupling various software modules is paramount to unveil the underlying physics and thus leads to an improved design of equipment and a more efficient operation. These simulations are in general to be carried out on small to massively parallelised computers for which highly efficient partitioning techniques are required. An innovative partitioning technology is presented that relies on a co-located partitioning of overlapping simulation domains meaning that the overlapping areas of each simulation domain are located at one node. Thus, communication between modules is significantly reduced as compared to an allocation of overlapping simulation domains on different nodes. A co-located partitioning reduces both memory and inter-process communication.

1 INTRODUCTION

Particulate materials and their thermal processing play an extremely important role in the worldwide manufacturing industry and are as diverse as pharmaceutical industry. processing and chemical industry, mining, construction and agricultural machinery, metal manufacturing, additive manufacturing, and renewable energy production. Particulate materials are intermediates or products of approximately 60% of the chemical industry (Ingram and Cameron, 2008).

These applications require a coupling between discrete particles represented by the Discrete Element Method (DEM) and a fluid phase referred to as Computational Fluid Dynamics (CFD) through heat, mass and momentum exchange and thus, constitute a multi-physics and multi-scale coupled application. Over the last decades, sophisticated methods and tools for surface coupling of separate parallel codes have been developed, in particular for continuum mechanical fluid-structure interaction (FSI) (Götz et al., 2010; Shunji et al., 2014; Mehl et al., 2016). Atomistic scales have been successfully coupled to continuum scales, both in concurrent (Tadmor et al., 1996; Xiao and Belytschko, 2004; Fish et al., 2007; Knap and Ortiz, 2001; Miller and Tadmor, 2002; Belytschko and Xiao, 2003; Wagner and Liu, 2003) and hierarchical (Fish, 2009; Luo et al., 2009; Bensoussan et al., 1978; Sanchez-Palencia, 1980; Li et al., 2008) modes. For very small particles, for which the Lagrangian point particle method (LPP) (Balachandar and Eaton, 2010) is a valid approach, different methods have been proposed for "relatively" large particles (Deb and Tafti, 2013; Farzaneh et al., 2011; Sun and Xiao, 2015; Wu et al., 2018; Capecelatro and Desjardins, 2013). However, these methods have mainly been applied in pure fluid dynamics applications and still struggle with heat transfer (Liu et al., 2019), not to mention mass transfer as first principle transfer properties. Hence, coupling CFD and DEM at large scale has not been achieved, and represents a challenge (Belytschko and Xiao, 2003; Yang et al., 2019) due to the highly dynamic data dependencies and the fact that particles and fluid are coupled in the whole domain instead of only across a lower-dimensional surface as in FSI.

The use of coupling libraries is a straight-forward and promising approach to achieve robust and stable model component and software coupling in general. However, generic coupling libraries fail to address the problems induced by the CFD-DEM volume coupling efficiently:

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LIME (Belcourt et al., 2011) has its dominant applications in the nuclear reactor modeling; *CASL* (Kothe, 2012) and *MOOSE* (Gaston et al., 2009) apply the Jacobian-free Newton Krylov (JFNK) method to handle multi-physics applications in a tightly coupled mode; *OASIS* (Valcke, 2013) and *MCT* (Larson et al., 2005) are dedicated to climate modeling including earth, ocean or atmosphere; the *Functional Mock-up Interface* (*FMI*) system (Blochwitz, 2014) has been initiated by Daimler AG to exchange simulation models between Original Equipment Manufacturers (OEMs) and suppliers, but does not support explicit parallelism; *MpCCI* (Joppich and Kürschner, 2006) is a commercial tool to couple various simulation software, but its centralized design represents a bottleneck for communication. Similarly, *ADVENTURE* (Shunji et al., 2014) and *EMPIRE* (emp,) have limited parallel scalability.

However, high performance computing (HPC) is a critical component to resolve the underlying multiphysical characteristics accurately within short computational times. Recent efforts achieved a scale-up of CFD-DEM coupled simulations to many hundreds of cores, but experience a considerable communication overhead. While some interfaces are available for coupling *Fluent* and *EDEM* (Spogis, 2008) and *LAMMPS* with *OpenFOAM* (Phuc et al., 2016; Foundation,), they offer very limited parallelization capabilities. A parallelized coupling for pharmaceutical applications has been undertaken between FIRE and XPS as proprietary software (XPS,), but is restricted to running XPS on GPU and FIRE on CPU architectures, respectively. In (Gopalakrishnan and Tafti, 2013), the authors developed a DEM solver within their multiphase flow (CFD) solver *MFIX*. Their scalability for up to 256 cores indicates an increase of communication overhead by 160% between 64 and 256 cores. (Sun and Xiao, 2016) shows the result of *SediFoam*, an ad-hoc coupling between *OpenFOAM* (for CFD) and *LAMMPS* (for DEM). Also their approach is limited by the communication overhead, which grows by 50% between executions from 128 to 512 cores. These performance issues are attributed to the large amount of data that needs to be exchanged between the CFD and DEM simulation domains due to the volume coupling.

Available massively parallel coupling libraries are *OpenPALM*, *CWIPI* and *preCICE*. *OpenPALM*, *CWIPI* (Buis et al., 2006; Piacentini et al., 2011) and MUI (Tang et al., 2015) have been used successfully for volume coupling (Boulet et al., 2018; de Laborderie et al., 2018). However, very few adapters for single physics software are publicly available. *preCICE* (Gatzhammer et al., 2010; Bungartz et al., 2016) implements fully parallel coupling numerics and point-to-point communication. While *preCICE* was primarily designed for surface coupling as used in fluid-structure interaction (FSI) (Mehl et al., 2016), recent work, has shown successful results for volume coupling (Arya, 2020; Besseron et al., 2020).

A common drawback of the existing approaches for partitioned volume coupling is that they are based on the existing domain partitioning within each single solver. This results in the above-mentioned huge amount of communication as inter-solver communication is not considered in the target function of the respective partitioning methods. To eliminate this issue, approaches for common domain partitioning over the entire domain of coupled solvers are required, and should be combined with sophisticated scheduling and load balancing methods within and across the computing nodes.

First ideas to address the issue of joint partitioning over several solvers based on graph partitioners, but limited to surface coupling, have been presented in (Predari, 2016; Predari and Esnard, 2014). Therefore, this contribution describes the so-called co-located partitioning approach for a volume-based coupling meaning that an exchange takes place within the entire simulation domain as opposed to boundaries only. Co-located partitions result from a partitioning of the entire simulation domain composed of the single-physics simulation domains. Consequently, simulation domains of each module overlap on one node, and thus reduce both memory and inter−process communication.

2 METHODOLOGY

Nowadays, software for both continuum and discrete mechanics has reached a degree of maturity that makes it a valuable tool for science and engineering in the respective domains. In order to address complex simulations in a discrete-continuous environment, two major approaches exist for coupling model components:

- In the monolithic approach, the equations describing multi-physics phenomena are combined in a large overall system of equations and solved by a single targeted solver. This requires implementing a new simulation code for each combination. Very often a new numerical solver has to be developed involving a dedicated pre-conditioner for the respective large and in general ill-condition system.
- In a coupled approach, appropriately tailored solvers for each physical domain are linked to

an overall simulation environment via suitable communication, data mapping and numerical coupling algorithms. This inherently encompasses a large degree of flexibility by coupling a variety of solvers. Furthermore, a more modular software development is retained, that allows applying established and highly efficient solvers for each physics addressed.

As outlined above, a coupling of "best-of-the-classes" software modules is preferred rather than implementation of additional features in an already available module. For this work, we will focus on the coupling of three software modules, XDEM represents the extended discrete element method, OpenFoam describe the fluid dynamics and deal.II (Arndt et al., 2021) is a finite element code. Based on first principles the data exchange between the modules covers momentum, heat and mass transfer. A common feature for the coupling strategies considered is that there is a large overlap between the individual domains shown in Figures 5 and 8. In both cases the particle domain covers also the CFD domain so that an exchange of momentum takes place not only on boundaries like in FSI but within the entire CFD and DEM simulation area. In particular, the dam break case with app. $2.35 \cdot 10^6$ particles and 10^7 CFD cells requires an intensive exchange of data between the CFD and particle domain.

In order to evaluate the momentum exchange i.e. drag forces acting on particles, fluid density, viscosity, specific heat, conductivity, and velocity components have to be transmitted to the particle domain commonly referred to as scalar, vector and tensor fields. Thus, each particle generates a momentum source for the flow fields that requires a transfer of the implicit and explicit part of the momentum source in conjunction with the void fraction. If in addition, heat and mass transfer have to be taken into account, fluid temperature and composition referring to species mass fractions also have to be provided. Exchanging this huge amount of data on massively parallel systems may lead to an unwanted side effect that communication between nodes may turn out as bottleneck for scalability as reported by (Gopalakrishnan and Tafti, 2013) and (Sun and Xiao, 2016). This immense communication overhead results from a "simple" coupling of modules for which a data transfer has not been taken into account as is sketched in Figure 1.

Almost every CFD and DEM solver comes with parallelisation capabilities that allow to run large cases on massively parallel systems. For this purpose, each software platform provides sophisticated partitioning techniques tailored for the particular application in mind that allows an efficient throughput

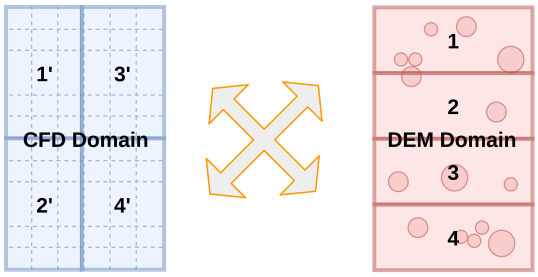

Figure 1: A "simple" coupling between a CFD and DEM module usually results in a large communication overhead due to individual solver strategies.

on HPC machines. In order to reach best performance and scalability, each software module follows its own strategies which most of the times do not consider communication between individual modules. Hence, a constellation as shown in Figure 1 occurs, in which each solver applies its individual partitioning independent of each other that generates a large communication overhead and might even lead to unpredictable or unphysical behaviour. However, the co-located partitioning technique (Pozzetti et al., 2018) offers a remedy to the unfavourable communication overhead and is based on the principles depicted in Figures 2 and 3.

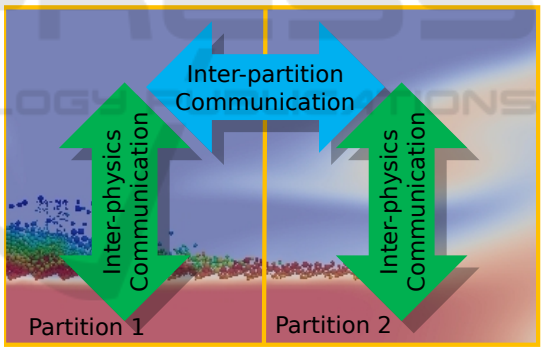

Figure 2: Distinction between inter-physics and inter-partition communication ina co-located partitioning.

The simulation domains in Figure 2 include a flow and motion of particles due to drag forces. An inter-physics communication takes place between the particles and the flow meaning that physical quantities as detailed above have to be exchanged to represent the physics between particles and flow. Consequently, the partitions of the particle module and flow module have to overlap as much as possible as depicted Figure 3, so that the inter-physics communication is kept within the same node. In an ideal arrangement, the particle and flow partition are identical.

Hence, the vast amount of data exchange occurs within the node for co-located partitions and a min-

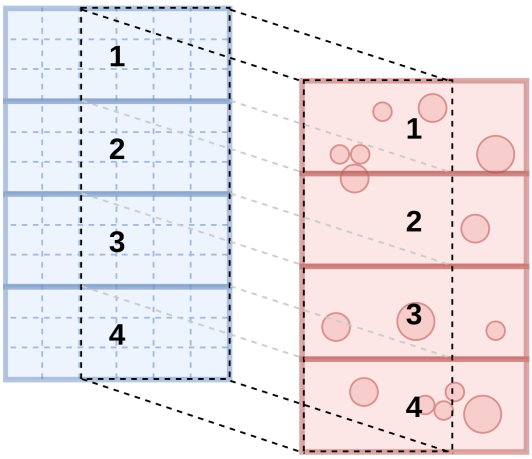

Figure 3: Largely overlapping partitions for a particle and CFD domain and, thus reducing communication significantly as compared to a "simple" partitioning based on individual solver strategies shown in Figure 1.

imum of data has to be communicated between the partitions for both particles and flow which leads to a significant reduction of the otherwise large communication overhead.

3 APPLICATIONS AND RESULTS

The co-located partitioning technology (Pozzetti et al., 2019) was applied to a dam break with debris e.g. particles as depicted in Figure 5 representing the initial conditions.

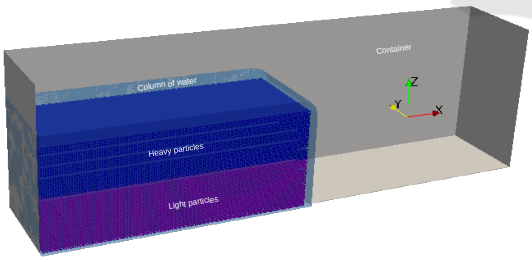

Figure 4: Dam break as a benchmark including 10^7 CFD cells and $2.35 \cdot 10^6$ particles.

A column of water contains particles of which app. half the number is lighter than water and the remaining particles are heavier than water. Initially, the heavier particles are located above the lighter particles so that an intensive mixing and therefore, relocation of particles takes place due to buoyancy forces. Thus, the heavy particles sink to the bottom while the light particles float and gather on the surface. This rearrangement of particles is superseded by the breaking water carrying particles due to drag forces. A snapshot of the configuration in motion is shown in Figure 5 in which particles undergo a rapid motion and the water experiences the typical breaking wave pattern at the right wall.

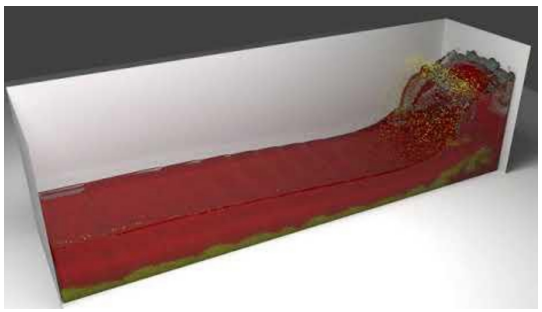

Figure 5: Snapshot of a water column enriched with particles breaking at a wall.

The above-mentioned results were obtained by coupling the Extended Discrete Element Method (XDEM) (Peters, 2013) [1] and OpenFoam [2] as CFD solver. For detailed information on the simulation platforms, the reader is referred to the respective internet pages (see footnotes) and the links provided herein. The data exchange included the variables as afore-mentioned and is schematically depicted in Figure 6.

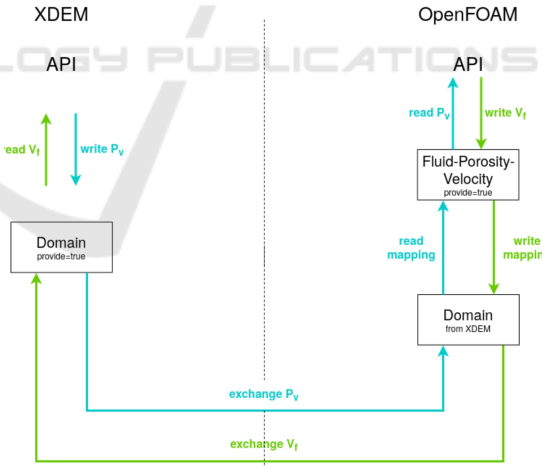

Figure 6: Data exchange between XDEM and OpenFoam labelled as 4-way-coupling.

Data between the CFD and particle domain is communicated in both directions indicated by the blue line for data travelling from the CFD domain to the particle domain. It includes the fluid properties required to evaluate the drag forces acting on particles.

[1] https://luxdem.uni.lu
[2] www.openfoamwiki.net

These drag forces represent a momentum source for the Navier-Stokes equations solved for in OpenFoam and is transferred to the CFD domain into the opposite direction represented by green lines. These quantities are all available on a co-located partition through direct memory access and therefore, do not require any effort for communication. In a "simple" coupling, these information is more than likely to reside on an other node which then would require additional and non-negligible communication that is avoided altogether within the proposed co-located partitioning. Only a minimum of communication is necessary between the partitions that covers both fluid and particle properties. Hence, a good scaleability is achieved and is shown in Figure 7.

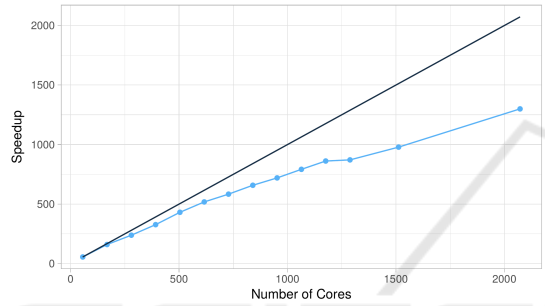

Figure 7: Speed-up versus number of cores for dam break benchmark.

For this purpose, the dam break case was executed on the HPC cluster [3] of the University of Luxembourg that allowed using up to app. 2000 cores. Under these initial conditions, a scalability of already 63 % was achieved which amounts to only 2.3 % of communication overhead. This technology is equally well applicable to more complex coupling scenarios as shown in Figure 8 in which three domains namely fluid flow, motion of particles and deformation of structures is considered.

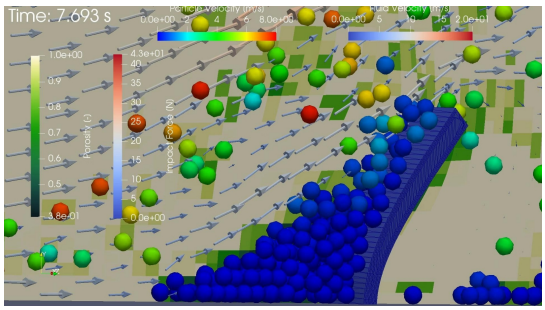

Figure 8: Predicted results of particle motion, flow and deformation by the modules of XDEM, OpenFoam and deal.II, respectively.

Similarly to the dam break case, the particle domain includes heavier and lighter particles than the fluid and thus, introducing buoyancy effects in addition to drag forces. Both, the particle and fluid simulation domain interact with a flap through forces. The fluid drag exerts forces on the flap, which itself causes the fluid to develop a recirculation zone behind the flap. Similarly, the particles generate impact forces on contacting the flap which leads to a considerable deformation of the flap due to fluid and particle forces. Particles in contact with the wall are stopped and sliding down on the wall surface due to dominating gravity. Hence, particles pile up in front of the wall and, thus, having a further impact on wall deformation and fluid flow. Similarly, particles reaching the wake region of the flow behind the flap form a pile due to gravity and negligible drag forces at much reduced flow velocities. Compared to the previous benchmark of the dam break, a coupling of three solver domains requires a more sophisticated coupling and communication of data structures and properties. Hence, in addition to the data exchange between OpenFoam and XDEM in Figure 6, both modules exchange data i.e. forces with the finite element module deal.II depicted in Figure 9.

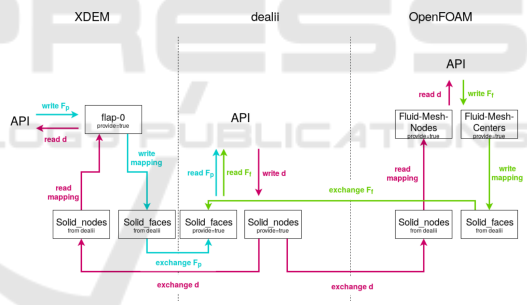

Figure 9: Data exchange between the modules of XDEM, OpenFoam and deal.II labelled as 6-way-coupling.

deal.II [4] is included as an additional simulation module to OpenFoam and XDEM. It is a finite element solver and predicts the deformation of the flap due to impact forces from the fluid and the particles. In addition to the aforementioned data exchange between the fluid and particle domain (blue and green lines) in Figure 6 both fluid and particle domain interact with the structural domain i.e. flap and introduce further communication lines between the modules (red lines). In order to evaluate an impact between the particles and the flap structure, geometry data is exchanges that allows determining the point of contact between a particle and the flap. The contact force resulting from the impact is predicted in con-

[3] https://hpc.uni.lu/

[4] www.dealii.org

junction with material exchanged properties of both the particle and the flap e.g. Young's modulo and Poison ratio for simple linear Hooke-like material behaviour. The predicted impact force leads to deformation of the flap and governs among other contact forces between particles and gravity the trajectory of particles. Similarly, the fluid pressure on the flap's surface generates a surface load contributing to further deformation of the flap.

Hence, a well coordinated and efficient data transfer between simulation domains allows investigating complex multi-physics and multi-scale in space and time applications. An analysis of predicted coupled results unveils the underlying physics acting inside the domains and between the domains. It provides an insight of unprecedented quality and is the key to an improved design of equipment and more efficient operation. The communication pattern, however, grows exponentially with each added module and therefore, requires an additional framework to coordinate the the communication lines correctly between the solvers. Additionally, data is to be exchanged at consistent times during iterations so that conservation principles are obeyed and physical laws are satisfied.

4 CONCLUSIONS

The demand for multi-physics applications be it multi-phase reacting flows as addressed in the current contribution or inn addition combined fluid dynamics under electro-magnetic influence such as magneto-hydrodynamics or electro-/magneto-rheological fluids (ERFs/MRFs) has grown substantially. A multi-physics simulation environment is achieved through two major concepts:

- Monolithic concept: The equations describing multi-physics phenomena are solved simultaneously by a single solver producing a complete solution.
- Staggered concept: The equations describing multi-physics phenomena are solved sequentially by appropriately tailored and distinct solvers with passing the results of one analysis as a load to the next.

The former concept requires a solver that includes a combination of all physical problems involved, and therefore, requires a large implementation effort. However, there exist scenarios for which it is difficult to arrange the coefficients of combined differential equations in one matrix. A staggered concept as a coupling between a number of solvers representing individual aspects of physics offers distinctive advantages over a monolithic concept. It inherently encompasses a large degree of flexibility by coupling an almost arbitrary number of solvers. Furthermore, a more modular software development is retained that allows by far more specific solver techniques adequate to the problems addressed. However, partitioned simulations impose stable and accurate coupling algorithms that convince by their pervasive character.

The exchange of data between different solvers requires a careful coordination and a complex feedback loop so that the coupled analysis converges to an accurate solution. This is performed by coupling algorithms between the Discrete Particle Method to the Finite Volume e.g. Computational Fluid Dynamics and the Finite Element Method e.g. structural engineering for which two fundamental concepts are employed:

- An exchange of data at the boundaries between discrete and continuous domains which represents at the point of contact a transfer of forces or fluxes such as heat or electrical charge.
- An exchange of data from particles submerged in the continuous phases into the continuous domain by volumetric sources.

The former defines additional boundary conditions, while the latter coupling appears as source terms in the relevant partial differential equations. Hence, applying appropriate boundary conditions and volumetric sources for the discrete and continuous domain furnishes a consistent and effective coupling mechanism.

However, the latter exchange of data impact parallel performance crucially. Not only that a data exchange over the entire simulation domain constitutes a huge amount of data transfer, it also generates a large communication effort. In order to reduce the communication to a minimum, a co-located partition strategy for coupling a number of solver modules has been proposed. Thus strategy places the partitions of the solvers on the same node so that the inter-physics exchange of data between the solvers occurs locally without inter-node communication. The latter is reduced to a minimum necessary to maintain the required communication between nodes.

Hence, inter-physics communication that otherwise has to travel between nodes is reduced significantly which is a fundamental step toward the large-scale computation in an high performance computing environment with hundreds of computing processes. Consequently, rather than carrying out the partitioning of the simulation domains by each solver independently and following its own requirements for performance, an overall partitioning strategy has to be applied. This includes dedicated partitioning algorithms

that identify a trade-off between communication requirements within the simulation domains and load-balancing so that the overall execution time is minimised.

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