First International Conference Math 2 Product (M2P 2023)
Emerging Technologies in Computational Science
for Industry, Sustainability and Innovation
May 30th - June 1st, 2023, Taormina, Italy

TOWARD HIGH-PERFORMANCE MULTI-PHYSICS COUPLED SIMULATIONS FOR THE INDUSTRY WITH XDEM

Xavier Besseron, Prasad Adhav, Daniel L. Louw, Bernard Peters

University of Luxembourg
2, avenue de l'Université
L-4365 Esch-sur-Alzette, Luxembourg
firstname.lastname@uni.lu
https://luxdem.uni.lu/

ABSTRACT

Computational simulation is an essential tool for researchers and scientific engineers to set up and explore experimental processes. Industrial applications drive the need for larger models and finer accuracy that require an increased amount of computation which motivates the use of High-Performance Computing (HPC) platforms to perform the simulations.

In our work, we focus on multi-physics simulations with particle-fluid interactions. We developed the XDEM (eXtended Discrete Element Method) framework [1] which simulates the motion and thermodynamic state of particles, and is coupled with independent Computational Fluid Dynamics (CFD) solvers for the simulation of fluids. This coupled multi-physics solution has successfully been used in a wide variety of industrial applications to simulate biomass combustion [2], blast furnace reduction processes [3] or abrasive water jet cutting [4]. In this presentation, we give an overview of the different techniques used in the XDEM software to simulate complex industrial processes on HPC platforms and how we make it available seamlessly to users:

The coupling between the particles and fluid phases is designed to be flexible and follows a modular design in which each component is replaceable. In this approach, the particle phase is represented in the fluid domain by field values (e.g. porosity, heat and mass sources) [5] that are added to the CFD models. It relies on the preCICE coupling library [6] which is responsible for the data mapping, interpolation and communication.

Because the coupling of particles within a fluid is a volume coupling (as opposed to surface coupling), it requires a significant amount of data to be exchanged. To address this issue, we have designed coupling-aware partitioning strategies that account for the workload and data distribution of all participants in order to reduce inter-process communication [7]. In Fig. 1, this approach is illustrated for a biomass furnace simulation.

Finally, we developed an automated scientific workflow to simplify the execution of these coupled simulations for non-HPC-expert end-users. Based on an all-in-one Singularity image, it takes care of all the steps: preparation of the input, execution on an HPC platform, and analysis of the results [2]. This workflow has been *cloudified* as part of the CloudiFacturing project [8].

With these developments, we put together the bricks necessary to provide flexible and turnkey multi-physics coupled simulation for industrial end-users that leverage the performance of HPC platforms.

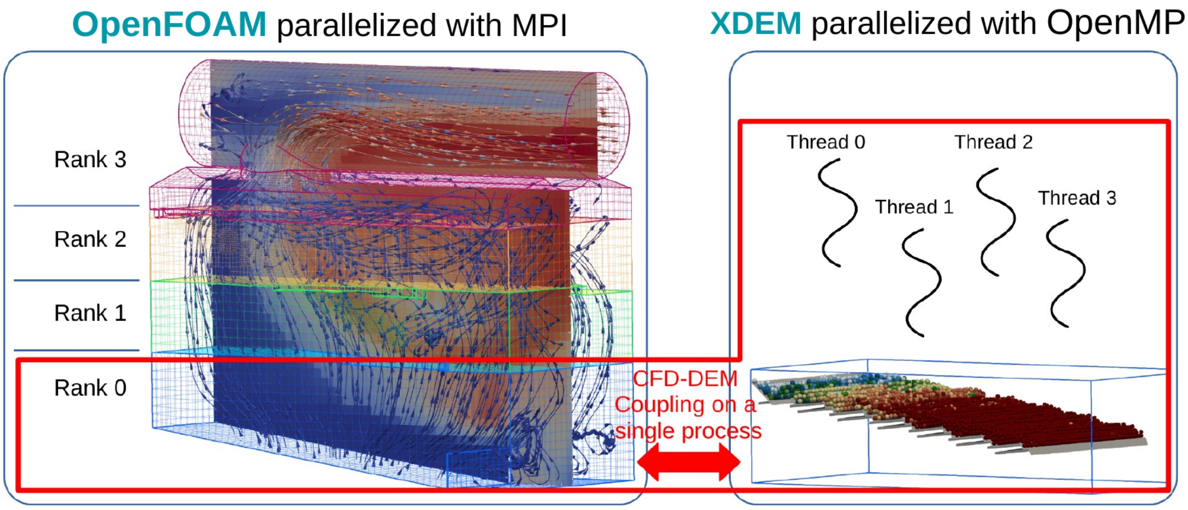

Fig 1. For the multi-physics simulation of a biomass furnace with OpenFOAM and XDEM, we developed a dedicated co-located partitioning approach that accounts for the spatial locality of the data between the two solvers in order to reduce the communications [2].

REFERENCES

[1] B. Peters *et al.*, "XDEM multi-physics and multi-scale simulation technology: Review of DEM–CFD coupling, methodology and engineering applications," *Particuology*, vol. 44, pp. 176–193, Jun. 2019, doi: 10.1016/j.partic.2018.04.005.

[2] X. Besseron, H. Rusche, and B. Peters, "Parallel Multi-Physics Simulation of Biomass Furnace and Cloud-based Workflow for SMEs," in *Practice and Experience in Advanced Research Computing (PEARC)*, Boston, MA, USA, Jul. 2022, pp. 1–9. doi: 10.1145/3491418.3530294.

[3] N. Aminnia *et al.*, "Three-dimensional CFD-DEM simulation of raceway transport phenomena in a blast furnace," *Fuel*, vol. 334, p. 126574, Feb. 2023, doi: 10.1016/j.fuel.2022.126574.

[4] P. Adhav, X. Besseron, A. Rousset, and B. Peters, "AWJC Nozzle simulation by 6-way coupling of DEM+CFD+FEM using preCICE coupling library," presented at the IX International Conference on Computational Methods for Coupled Problems in Science and Engineering (COUPLED 2021), Online, Jun. 16, 2021. [Online]. Available: https://precice.org/eccomas-coupled-2021.html

[5] B. Peters, X. Besseron, A. Peyraut, M. Mehl, and B. Ueckermann, "An Innovative Partitioning Technology for Coupled Software Modules," in *Proceedings of the 12th International Conference on Simulation and Modeling Methodologies, Technologies and Applications (SIMULTECH)*, Lisbon, Portugal, Jul. 2022, pp. 186–193. doi: 10.5220/0011135200003274.

[6] G. Chourdakis *et al.*, "preCICE v2: A sustainable and user-friendly coupling library," *Open Res. Eur.*, vol. 2, p. 51, Sep. 2022, doi: 10.12688/openreseurope.14445.2.

[7] G. Pozzetti, H. Jasak, X. Besseron, A. Rousset, and B. Peters, "A parallel dual-grid multiscale approach to CFD–DEM couplings," *J. Comput. Phys.*, vol. 378, pp. 708–722, Feb. 2019, doi: 10.1016/j.jcp.2018.11.030.

[8] T. Kiss, "A Cloud/HPC Platform and Marketplace for Manufacturing SMEs," presented at the 11th Int. Workshop on Sci. Gateways (IWSG), Slovenia, May 2019. Accessed: Oct. 06, 2021. [Online]. Available: http://www.iwsg2019.eu/