HPC LARGE SCALE SIMULATION OF AN INDUSTRIAL FLUIDIZED BED AND APPLICATIONS TO CHEMICAL ENGINEERING PROCESSES WITH NEPTUNE_CFD

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Fluidized beds and more broadly dilute and dense particle-laden reactive flows are encountered in a wide range of industrial chemical engineering applications such as catalytic polymerization, coal combustion … Nowadays, it is possible to perform realistic 3D simulations of industrial configurations using an unsteady Eulerian multi-fluid approach for polydisperse reactive flows with a good physical modelling. Hence CFD is a powerful tool for studying the optimization of chemical processes, new designs and scaling-up.

To obtain numerical results in an acceptable CPU time, it is important to check the feasibility of CFD simulation of fluidized bed flows in complex geometries at industrial scale. Also we need to estimate HPC capacities of CFD tools. Numerical simulations have been performed with the solver NEPTUNE_CFD: parallelized unstructured code (MPI) using unsteady Eulerian multi-fluid approach. NEPTUNE_CFD is based on the same numerical methods than Code_Saturne. Code_Saturne is an open source CFD software code ready to run on petascale machines. NEPTUNE_CFD's high parallel computing performances for particle-laden flows have been demonstrated over last years. Recent developments allow overtaking NEPTUNE_CFD's limitations making it fit for massive parallel computing.

In the present study, the massively parallel computing performances of NEPTUNE_CFD are investigated. We show the results of a numerical simulation of a 3D dense fluidized bed reactor at industrial scale including more than 80 tons of particles. The geometry is about 5 meters in diameter and 30 meters in height. The mesh has more than one hundred million hexahedral cells leading to cells of $1cm^3$. The parallel numerical simulation has been performed using up to 12 000 cores on a massive parallel supercomputer. This kind of very large simulation is able to capture the different scales of such a complex multiphase flow: from the large flow structures to the small ones (particle clusters, bubbling …). It is important to capture these small structures as they are essential features of reactive flows. The results of this study constitute a reference for the development of sub-grid models to be used on coarser meshes.

We also focus on reactors featuring rotating parts. They are common in chemical engineering processes. It is essential to take these rotating parts into account, even with complex industrial geometries, as they enhance chemical reactions. NEPTUNE_CFD's rotating mesh numerical methodology is now effective. The method is based on splitting the domain into static and rotating parts and information is passed thanks to a non-conformal mesh matching technique. Methodology and numerical results are presented.

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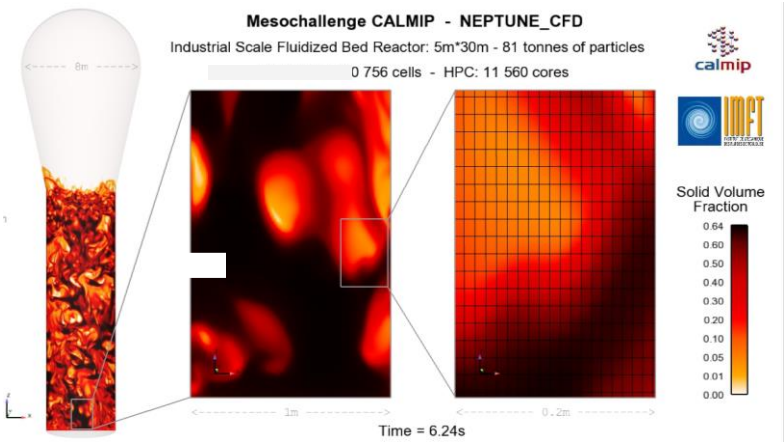

Figure 1 - NEPTUNE_CFD simulation of an industrial 3D fluidized bed reactor