Lethe: Massively Parallel Open-source Multiphase CFD for the Simulation, Design, and Optimization of Unit Operations
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Chemical process plants generally consist of a combination of multiple unit operations which all have a specific purpose: separating components, facilitating a chemical reaction, mixing, transferring energy from one fluid to another, moving fluids. The design of these operations is still mostly based on design heuristics which lead to significant challenges when designing new chemical processes or scaling-up existing ones. These challenges are exacerbated by the occurrence of turbulence, the complex rheology of the fluid or the presence of multiple phases such as a fluid (gas or liquid) and solid particles. Computational Fluid Dynamics (CFD) for the fluid phase, the Discrete Element Method (DEM) for granular material, and their combination (CFD-DEM) enable us to predict the dynamics of these unit operations. This requires high-performance robust models for which the components (linear solver, finite element formulation) are tailored to the application.

In this talk, we introduce a new open-source CFD, DEM and CFD-DEM software: Lethe. Lethe is built upon the well-established deal.II library. It leverages deal.II not only for its state of the art FEM capabilities, but it also makes extensive usage of its high-performance particle tracking module for its DEM solver. We present different examples that highlight the challenges that the chemical engineering community face and that can be addressed through simulations such as the mixing of complex fluids, the prediction of multiphase flows in rotating packed bed reactors, the flow in spouted and fluidized bed reactors, etc.

For each of these examples, we discuss the mathematical formulation that we use within Lethe as well as the technical challenges faced when developing the models. We conclude by providing a high-level perspective of the direction in which we are heading, the challenges that we are currently facing and the key lessons that have been learned through this endeavor to develop an open-source CFD/DEM/CFD-DEM software.