ParScale - An Open-Source Library for the Simulation of Intra-Particle Heat and Mass Transport Processes in Coupled Simulations

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ABSTRACT

Dense particle laden flows are encountered in a wide range of engineering applications, including chemical and pharmaceutical engineering. In order to simulate these particle systems, Discrete Element Method (DEM) and Computational Fluid Dynamics-DEM tools became state of the art over the past ten years [1]. These tools provide a detailed understanding of the flow behavior, and are able to resolve phenomena on a particle level with high computational efficiency [2]. At the moment, these tools do not take intra-particle phenomena, e.g., a non-uniform temperature profile inside each particle, into account. Unfortunately, spatially resolved intra-particle properties are of key importance in reactive systems [3]. Hence, there is a need to establish software tools that can be linked to existing DEM codes to resolve intra-particle properties if needed.

The newly developed library *ParScale* is developed in a C/C++ environment and publicly available. It is designed for spherical particles with a fixed number of intra-particle mesh points, and a one-dimensional discretization. Various models are available within *ParScale*, e.g., heat and mass transfer models, grain-scale models, as well as single reaction and multiple heterogeneous reactions. The modular class based structure ensures easy extendibility. Also, *ParScale* is embedded into an automated test harness to ensure software quality.

With the current state of *ParScale* it is possible to resolve species and temperature profiles in coupled simulations (using the DEM code LIGGGHTS), or as a stand-alone tool. The effect of these profiles is demonstrated for the case of heat transfer at high Biot numbers in a sheared particle bed. Development and testing of *ParScale* is still ongoing and preliminary results of benchmarking studies with respect to parallel performance will be presented as well.

REFERENCES

[1] C. Kloss, C. Goniva, A. Hager, S. Amberger, S. Pirker (2012) "Models, algorithms and validation for opensource DEM and CFD-DEM", Progress in Computational Fluid Dynamics, Vol. 12, Nos. 2/3, pp. 140-152.

[2] C. L. Wu, O. Ayeni, A.S. Berrouk, K. Nandakumar (2014) "Parallel algorithms for CFD–DEM modeling of dense particulate flows", Chemical Engineering Science, Vol. 118, pp. 221-244.

[3] A. G. Dixon, M. E. Taskin, E. H. Stitt, M. Nijemeisland (2007) "3D CFD Simulations of Steam Reforming with Resolved Intra Particle Reaction and Gradients", Chemical Engineering Science, Vol. 62, pp. 4963-4966.