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Modelling of Multiphase Flow in Process Equipment: The Trade-off between Accuracy and Computational Efficiency

Wednesday, 6 December 2017 13:30 (30 minutes)

Process equipment behaviour is characterised by multiscale multiphase interactions namely: liquid-gas, fluid-particle, particle-particle and particle-wall interactions. The understanding of these interactions, ideally, requires a general solution to the full turbulent Navier-Stokes equations combined with a unifying theory for granular flow. However, in the absence of such breakthroughs advances in Computational Fluid Dynamics (CFD) and Computational Granular Dynamics (CGD) are essential.

It is evident from the literature that significant advances in the theory of fluid and granular dynamics has had a positive bearing on the advancement of the industrial value of chemical, metal and mineral processing industries [1,2,3]. According to Joshi and Ranade [1] CFD is a technology that can be used to achieve these advances from the fluid dynamics perspective. In the same light, Pschel and Schwager [3] assert that computational granular dynamics (CGD) is also necessary to achieve these advances. Based on the advances in both fields it is clear that a combination of both is required to make the necessary leaps in technology required to achieve the above. However, the combined modelling of the complex physics is often computationally intensive, leaving the practitioner with the trade-off between the accuracy of the model predictions and the computational efficiency of the model.

The aim of this research is to improve the understanding of the physics of such flows and to provide accurate and computationally efficient models to be used in design optimisation of mineral processing processes and equipment. Currently hydrocyclones have been used as the examplar. However, broader applications are being introduced. Multiple vartiations of Navier-Stokes and Lattice Boltzmann Method (LBM) based models, coupled with the Discrete Element Method (DEM), are employed in the research. The models are benchmarked against experiment to determine accuracy and also benchmarked against each other for computational efficiency.

The major contribution of this research is the demonstration that the LBM can provide predictions of the multiphase flow and interactions in a hydrocyclone that are at least comparable to, and in some cases superior to, the Navier-Stokes based approach whilst remaining more computationally efficient (or comparable) to the Navier-Stokes based approach. Future work will focus on the development of a stable two-fluid LBM model and coupled a LBM-DEM model.

[1] J. B. Joshi and V. V. Ranade, "Computational fluid dynamics for designing process equipment: expectations, current status, and path forward," Industrial & Engineering Chemistry Research, vol. 42, pp. 1115–1128, 2003.

[2] H. E. Van den Akker, "Toward a truly multiscale computational strategy for simulating turbulent two-phase flow processes," Industrial and Engineering Chemistry Research, vol. 49, pp. 10780–10797, 2010.

[3] T. Pschel and T. Schwager, Computational Granular Dynamics: Models and Algorithms, 1st ed. Heidelberg, New York: Springer-Berlin, 2005.

HPC content

The research is focused on the application of HPC. The codes used on the CHPC for this research are:

- ANSYS Fluent
- Palabos

The models make use of between 48 and 120 cores per simulation. The usual wall time per simulation is 10 hours +. MPI as well as a combination of MPI and OpenMP is used.

Primary author: Dr BHAMJEE, Muaaz (University of Johannesburg)

Presenter: Dr BHAMJEE, Muaaz (University of Johannesburg)

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