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Parallel, multi-scale, mechanistic model for high shear granulation using coupled DEM PBM models on high performance computing systems.

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Abstract

A multiscale model combines the computational efficiency of a macro-scale model and the accuracy of a micro-scale model. It is preferred over a fully micro-scale model for its speed advantages while maintaining the physics of the problem. A less accurate way to perform such a simulation is touse data from a precomputed microscale model in a macroscale model. With the current cyberinfrastructure resources available, using more computationally intensive and concurrent multiscale models are morefeasible. This study proposes to use Discrete Element Method (DEM), a microscale model, and a Population Balance Model (PBM), a macroscale model, in a concurrent manner to model the granulation process of a pharmaceutical product inside a high shear granulator. The granulation between the components of a pharmaceutical blend is governed by the collision in between the particles. This leads to increase in their size, due to physical bonds in between them. The DEM provides the collision data while the PBM helps in predicting the macroscale phenomena like aggregation and breakage. This work attempts to couple these two models using a controller program, which triggers the DEM first, to give initial seed data to run the PBM. Then, the controller uses the data generated from the PBM continuously to determine the change in the physical properties and trigger the DEM from its last known state. The controller does the same with the DEM data to trigger the PBM. This occurs iteratively until a steady state is reached. A workflow diagram of the procedure followed is provided in Figure 1. The execution of each of the components is governed by a multilevel job scheduler which allocates resources rather than waiting for each simulation to run on a normal job scheduler on a cluster. The DEM is parallelized using Message Parsing Interface (MPI) while the PBM is parallelized using a faster hybrid approach which is a combination of both MPI and Open Multi-Processing (OMP). Since the DEM is computationally heavy, an algorithm is developed to utilize the idle cores during the PBM execution to run multiple instances of the PBM such that parameter estimation of the kernels of the PBM occurs on the fly as well. This method of using shorter bursts of each simulation led to faster simulation times as well as a more accurate model of the high shear granulator. The Quality by Design (QbD) approach is addressed using such a modelling framework and it also helps us understand the granulation process in a quantitative as well as in a mechanistic manner. (Firstauthor and Secondauthor, 2015)

Keywords: Multi-scale Model, Population Balance Model, Discrete Element Method, High-performance computing, MPI

1. Introduction

- Talk about pharmaceutical processes
- Talk about DEM and PBM
- Coupling and its importance
- Advantages of using HPC

2. Methods

2.1. Population Balance Model (PBM) development

- Aggregation
- Breakage

2.2. Discrete Element Model (DEM) setup

2.3. PBM parallelization technique

2.4. Controller development

Explain the controller configuration and how it works

3. Results

Discuss how many instances of the simulation of each occured

3.1. Scaling results

Cores used for DEM and PBM and how scaling occured

3.2. Improved results over one way coupling

Better d50 plots particle count

4. Conclusion

References

A. Firstauthor, B. Secondauthor, 2015. Very important article. Journal of unviversal rejection 42, 1–99.