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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.

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

1. Introduction

Particulate materials are products or intermidiates of around 60% of the chemical industry(Ingram and Cameron, 2005). The modelling of these particulate processes pose a challenge when compared to modelling if uniform liquid systems. These solid systems usually comprise of solids which co-exist with various sizes and shape configuration, which have a large effect on the final composition and the performance of the product. This variation in the configuration of the product is unaccepatable by the pharmaceutical industry. It could lead to differences in the dissolution rates and bioavailability of the product thus, affecting the quality of the product. The unit process that helps control the size of a granule of the powder in the pharmaceutical product is granulation. During this unit operation, fine powders are converted to the larger particles by the process of aggregation. This occurs due to addition of a liquid binder, making the particles agglomerate into larger granules. This process is also referred to as wet granulation as a liquid binder is added. Due to high restrictions set by the Food and Drug Administration (FDA) these products undergo various batch rejections or have high recycle ratios(Sen et al., 2014). One of the major aims of the industry currently is to reduce this waste, thus creating a need for better modelling of this process.

The most popular way to model the granulation process is to use a population balance model (PBM). This model tracks the number of particles with certain set of charactersitics such as size, porosity and liquid content. It also takes into account the changes that may occur in these properties due to growth, breakage, consolidation, and other phenomena. This model is discussed in more detail in section 2.1. PBM fails to account for the particle level data, thus being inaccurate at times. This particle level data needed to improve the PBM can be obtained from discrete element methods (DEM). DEM help obtain the velocity of each particle and the number of times it collides with other particles by solving the Newton's laws of motion. This information is vital to the PBM as it helps develop a more accurate model with a higher physical significance. As these methods are complementary to each other, they are usually coupled whille building a model for the granulation process. These processes can be coupled serially like in **(cite current paper here)** or in parallel as discussed in this work. DEM is always executed at initiation and the particle level data is then transferred to the PBM. The DEM simulation is computationally very high as it needs to solve large amounts of simultaneous equations at every time step. The parallel execution of this type of coupling requires various instances of simulation of each of these models to be initiated, requiring high computational power. The most efficient way to make these simulations run faster is to take advantage of large number of CPU cores present on modern day high-performance computing systems (HPCs / supercomputers).

This work focusses on the building of physically accurate model for a high shear granulator. Section 2 discusses the model equation used and the method of parallelization implemented on the PBM and DEM to enable them to run on various cores of HPCs. The resulting particle properties from the coupling and the speed improvements achieved when the number of cores used for the simulation are changed, is discussed in section 3.

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

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