ESTIMATION OF NUMERICAL ERRORS RELATED TO SOME BASIC ASSUMPTIONS IN DISCRETE PARTICLE METHODS

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Summary

Discrete particle methods that track the motion of individual particles and their collisions are computationally very expensive. Some basic assumptions are commonly introduced in the literature in order to accelerate these numerical simulations. In this study the use of computational parcels, or clouds, wherein many particles are lumped together so that only parcels and their collisions are tracked is examined. The multiphase particle-in-cell, or MP-PIC, wherein the collision forces are replaced by a solids pressure term with the main purpose to avoid exceeding maximum packing of the granular assembly is also investigated. Several cases relevant to the fluidization community are studied and errors associated with these basic assumptions are computed. Errors in the time-averaged flow variables are large indicating that further research is necessary to validate these basic assumptions.

Keywords

Multiphase and particulate reactors.

Introduction

Particulate flows occur commonly in nature, such as dust storms and volcanic eruptions, as well as in many industries, such chemical and energy conversion technologies. Traditionally, two approaches have been used to model particulate flow systems. The first is based on granular kinetic theory[1,2], which treats the granular media as a continuum (also called Eulerian or two-fluid model). The second is based on discrete particle methods[3,4] (Lagrangian), which describes the motion of each individual particle following Newton's second law and resolves collisions between particles and wall boundaries using either a soft-sphere or a hard-sphere model. The discrete method is more accurate than the continuum description of particulate flows since it involves fewer assumptions in the model derivation. However, numerical simulations based on this method are extremely expensive for any practical system due to the large numbers of particles.

To avoid tracking large numbers of particles in a discrete particle simulation, researchers have employed the concept of computational parcels, or clouds, which contain many particles moving at the same velocity[5,8]. Such a concept is commonly used in discrete simulations of droplets to model sprays[6]. Although using computational parcels seems reasonable for dilute flow conditions where collisions are scarce, this technique has been extended to model fluidized beds where both collisions and fluid-particle interactions play a major role in the transport mechanisms of particles. In either case, the concept of computational parcels needs to be rigorously verified for as many practical applications as possible. Thus far, however, the literature studies have focused on qualitative validation of this approach using experimental data and/or observations[7-9]. Accordingly, the goal of the current study is to accurately verify the concept of computational parcels by comparing the numerical results obtained using different parcel sizes. The results using the smallest numbers of particles per parcels are assumed to be the most accurate, which provides a robust method to estimate the errors in simulations with larger numbers of particles per parcel. Two different test cases are examined. The first computational test case is a wall-bounded shear flow of particles in a vacuum, where the parcel size ranges from a single particle to 10 particles per parcel. All collision parameters are the same for different parcel sizes. Since collisions are the only mean of momentum and energy transport in this system, it can be considered as a worst case scenario for the parcel method. A second test case, more relevant to fluidization, involves the flow of air and particles in a periodic vertical riser. Similar to the first system investigated, simulations are conducted using several parcel sizes and the time-averaged results are compared in order to estimate the numerical errors associated with the computational parcel assumption. Although large computational parcels containing thousands of particles have been used in the literature[7-9], this current study shows that significant errors occur even

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with an order of magnitude increase in the number of particles per parcel.

In addition to studying the impact of the computational parcel assumption, the effect of a solids pressure gradient in the particle equation of motion in place of the traditional collision forces associated with soft-sphere and hard-sphere discrete models, is investigated. The continuum solids pressure is primarily employed to avoid exceeding the maximum packing of the granular assembly. This approach is commonly referred to as the multiphase particle in-cell (MP-PIC) technique[7,8,9,10] and also uses computational parcels as described earlier. To estimate the errors associated with the MP-PIC assumption, sets of discrete parcel simulations using either the solids pressure gradient term or the collision force based on a soft-sphere linear spring-dashpot model are conducted. The time-averaged flow profile results obtained using the MP-PIC model are compared to those obtained using the soft-sphere collision model. Differences between these results are considered to reflect the numerical error associated with the MP-PIC assumption. For this study, simulations of a bubbling fluidized bed and a periodic riser flow of 500-micron particles and air are conducted.

In this study, the numerical errors associated with the computational parcel assumption and the MP-PIC approach are summarized for several basic particle-air flow systems of interest to the fluidization community (e.g. bubbling and transport fluidized beds). While examining time-averaged flow variables, such as particles velocity, concentration, and granular temperature, large errors were calculated. The results suggest that further analysis and research are necessary to fully validate the basic assumptions used in these discrete methods.

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