An efficient algorithm for the detection of neighbouring particles: prediction of the behaviour of a bubbling fluidised bed

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Abstract

An efficient algorithm for particle–particle and particle–wall collision detection in the two-dimensional case is briefly presented. The algorithm ensures an efficient computation of colliding particle flows. The physical domain is hierarchically divided and structured as a quad-tree. The algorithm is intended for particle-laden flows, which require small time steps, but within each time step, the algorithm is event-driven. The algorithm is used here to study the flow behaviour of a laboratory-scale fluidised bed. The two-dimensional motion of each individual spherical particle is directed, calculated from the forces acting on it, accounting for the interaction between the particle and the gas phase. The soft sphere model is used in the present work. The contact forces are continuous and finite and are a function of the deformations of the particles. A comparison of experimental observations and computational results of a two-dimensional laboratory-scale bubbling fluidised bed is presented and discussed.

Keywords: Contacts detection algorithm; Soft sphere dynamics; Cell structure; Quad-tree; Particle-laden flow; Discrete element method

1. Introduction

During the past decade, the discrete element method (DEM), in which every single particle is tracked, has been used by many investigators and gives promising results [1–3]. There is still a long way to go before full-sized equipment containing 10^{12}–10^{15} particles can be simulated using the DEM, but meanwhile the DEM can give useful statistics for methods that handle the particles as a continuum and to improve the understanding on a mesoscopic level [4].

When the particle concentration is so high that the dynamics are dominated by several particles being in contact simultaneously, such as in fluidised beds or gravity settling, the soft sphere model should be used. A time-consuming part of a DEM using a soft sphere model for particle particle interaction is the calculation of the forces. A $O(N^2)$ search, where N is the number of particles, is reduced to $O(N)$ by using a cell structure [5].

An algorithm for simulating soft sphere particle dynamics in two dimensions, developed along the lines of Melheim and Gjetsvik [6], is employed. The algorithm uses a cell system for collision detection. In the present work, the algorithm of Melheim and Gjetsvik [6] is extended to handle finite-time collision models such as the soft sphere model. The numerical predictions are compared qualitatively with experimental observations of the bubble formation in a two-dimensional laboratory fluidised bed. A discussion about the obtained results and their discrepancies is presented.

2. Background

2.1. Particle physics

The trajectory of a discrete particle is calculated by integrating Newton's second law for the particle, which is written in a Lagrangian reference frame. The law equates the particle inertia with the forces acting on the particle, and can be written as:

$$\frac{d\mathbf{v}_d}{dt} = \mathbf{F}_C + \mathbf{F}_D + \mathbf{F}_G + \ldots \quad (1)$$

The particle velocity is denoted by $\mathbf{v}_d$, and forces

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Computational Fluid and Solid Mechanics 2005
K.J. Bathe (Editor)

acting on the particles may be contact forces $\mathbf{F}_C$, drag forces $\mathbf{F}_D$ or gravity $\mathbf{F}_G$. The forces $\mathbf{F}_i$ are given per unit mass. Similarly, the rotation rate of the particle may be determined from:

$$\frac{\boldsymbol{\Omega}_d}{dt} = \frac{\mathbf{T}_C + \mathbf{T}_f}{I_d} \tag{2}$$

where $\boldsymbol{\Omega}_d$ denotes the angular velocity of the particle around its mass centre, $\mathbf{T}_C$ denotes the torque due to contact forces, and $\mathbf{T}_f$ represents other field contributions. Additional forces may be incorporated when forces other than those due to contract, drag and gravity are of importance. In the present work, the soft sphere model of Cundall and Strack [7] is used. The contact forces are continuous and finite. They are a function of the deformations of the particles, and are modelled with a simple mechanical analogy involving a spring, a dash pot and a slider.

2.2. *Cell system for collision detection*

The most time-consuming part of a soft sphere or molecular dynamics code is the calculation of the forces. In principle, for a given particle, we have to check for possible contact with every other particle in the system. Scanning particles for possible contacts is very time-consuming when the number of particles is large, since it scales as N^2, where N is the number of particles. However, the short-range nature of the interaction makes it possible to reduce the contact checking to O (N), for example by employing a neighbour list. The spatial domain is partitioned into rectangular cells, and the idea is that if we keep track of which particles are in each cell, and if the cells are larger than the largest particle, then for each particle we need check only for contacts with particles in the neighbouring cells. The cell structure proposed by Melheim and Gjelsvik [6] is used in this paper.

2.2.1. *Algorithm for the particle model*

The outlines of the framework for the computation of the trajectories of the discrete particles are presented here. The algorithm uses the computational strategy of Hoomans et al. [2], where we have included the priority queue of particle events of Lubachevsky [8], the data structures of Sigurgeirson et al. [9], and the cell structure presented by Melheim and Gjelsvik [8].

The algorithm consists of three primary data structures:

1. *The particle information:* arrays with information about the particles, their positions, velocities, size, etc.
2. *The event queue*, which is a collection of events, each with an event time and information to carry out the event. In this queue, a maximum of one event is stored per particle. Possible events are:
   - a collision with another particle;
   - a wall collision;
   - a transfer (the particle moves to a neighbour cell);
   - a check (the particle is to be checked for new events);
   - the particle is to be removed, for instance when the particle hit an outlet.
3. *The cell structure*, which contains information to make a neighbour-particle list in an efficient way.

The primary data structure is maintained in the operations of the algorithm.

Fig. 1 shows the primary flow chart. Initially, at each time step counters are reset and if there are new particles to add, these are initialised and added. If the cell structure is chosen to be adaptive, cells are split and merged. Then the forces on the particles are recalculated based on an updated fluid velocity field. Based on the positions and velocities at the end of the previous time step, a new event queue is built.

The main loop is the engine of the algorithm. The events are handled, new events are detected, and cell

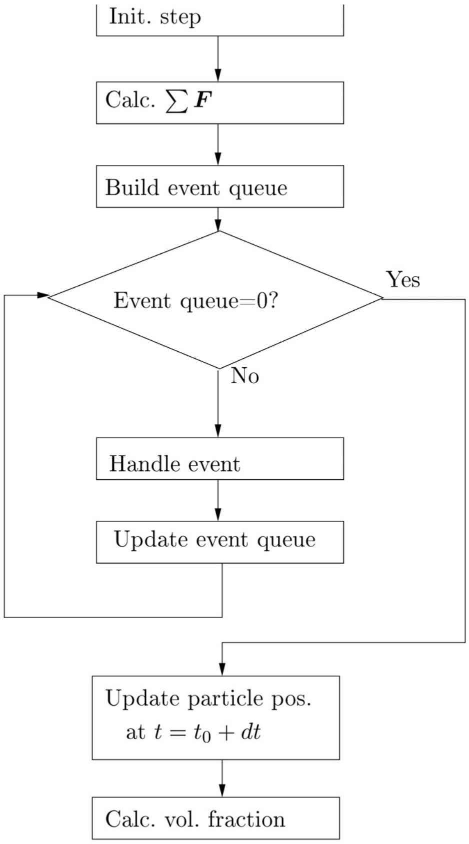

Fig. 1. Primary flow chart.

particle lists and the event queue are updated. The loop runs until no more events will happen during the time step [6]. During the time step, only particles that are in contact either with each other or with the wall are moved. At the end of the time step, the position of all particles is recalculated. Finally, particle–fluid cell mapping is updated and the volume fraction of particles in each fluid cell is calculated.

3. Experimental and numerical results

3.1. Experimental results

A two-dimensional fluidised bed with a central jet is constructed in order to study the bed expansion and bubble formation in gas–solid flow [4]. The purpose of this study is to verify the predictive capability of the DEM employed here. A digital video camera is applied to measure bubble formation and velocity.

Between 0 and 280 ms, the bubble size increases but is located at the approximate same vertical position (see Fig. 2). At time 280 ms, the bubble diameter is $d_b \approx$ 3.9 cm, and the bubble starts to rise. The bubble moves upwards and, maintaining a circular shape, its diameter increases to 7.5 cm during the next 320 ms. At this point, the bubble continues to move upwards, but its shape changes and bubble break-up is observed (Fig. 2). At time 320 ms, a new bubble is formed at the bottom of the bed and starts to rise. This new bubble differs significantly in shape from the first one and seems to remain attached to the bottom of the bed for the next 160 ms.

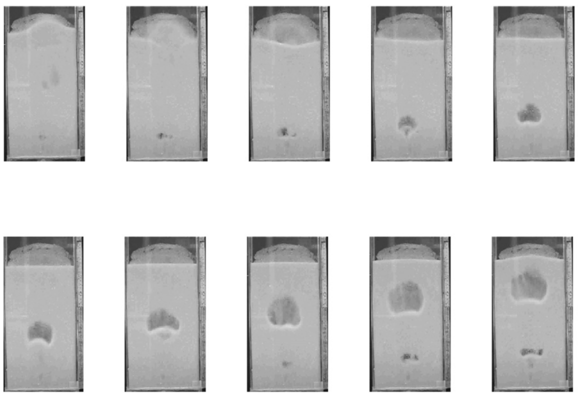

Fig. 2. Sequence of pictures of a two-dimensional fluidised bed. The time interval between each shot is $\Delta t = 80$ ms. In the first picture taken at time $t_0 = 120$ ms, an air bubble is about to appear.

3.2. Numerical results

Independence of the numerical results from the spatial discretisation is ensured for the simulations performed with the DEM. In the present work, a static cell structure with optimal size is preferred to an adaptive cell structure for the reasons pointed out by Melheim and Gjelsvik [6].

The restitution coefficient used in calculation performed in this work is $e_n = 0.95$. The particle density is $\rho = 2500\,\text{kg/m}^3$. Furthermore, a size distribution similar to that measured in the experiment is employed in our calculations.

Fig. 3 presents the prediction obtained from the DEM approach. Between 0 and 360 ms, the bubble size increases and rises in the vertical direction. The bubble remains attached to the bottom of the fluidised bed, where the air is injected. It elongates, assuming more and more an eliptical shape. At time 420 ms, the bubble leaves the horizontal plane and starts to move upwards. Its area increases during the next 320 ms, but it maintains the same shape. At this point, the bubble continues to move upwards, but its shape changes and bubble break-up is observed. A new bubble is formed and starts to rise at time 680 ms. The shape of this second bubble differs from that of the first one and is rather elongated. It remains attached to the bed for the next 160 ms.

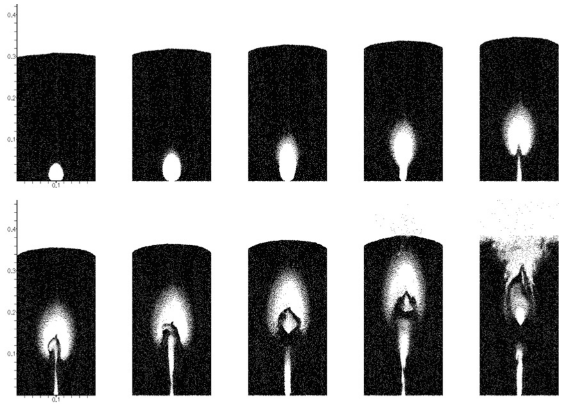

Fig. 3. Numerical prediction of a two-dimensional fluidised bed formulated with a Eulerian–Lagrangian approach. $\Delta t = 80$ ms is the time interval between each picture.

3.3. Discussion and final remarks

Figs 2 and 3 show a qualitative comparison between the experimental observations of the bubbling fluidised bed and the numerical results obtained with the DEM. In Fig. 4, the observed and predicted position of the first bubble is plotted as a function of time. A good

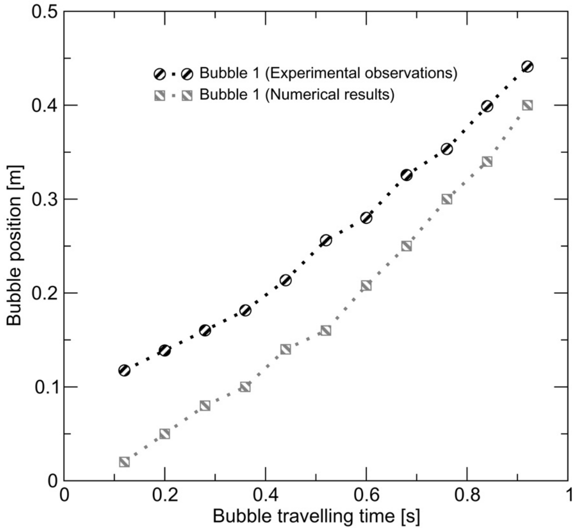

Fig. 4. The position of the first bubble in the bed is plotted as a function of time. Experimental observations are compared with numerical results.

agreement is observed. The shape of the bubble predicted numerically differs from the experimental observations, especially when the bubble is generated. The formation time and the shape of the second bubble also seem to be predicted well from the numerical calculation.

The overall behaviour of the fluidised bed predicted by the DEM simulation seems to be described in a satisfactory way.

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