Coupled CFD/DEM Simulations

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The coupling of computational fluid dynamics (CFD) and discrete element models (DEM) is increasingly popular to study fluid-particle systems, and possibly fluid-bubble systems as well. Discrete element models (DEM) have been used for a wide range of applications involving particles (*e.g.* Zhu et al. (2008)), ever ever since it was first proposed by Cundall and Strack (1979).

In DEM, the particle behaviour is resolved individually (per particle) and deterministically, by solving Newton's second law for each of the particles in the system. From a conceptual point this is straightforward, as there are many successful approaches in solving Newton's second law accurately. However, the challenge lies in the fact that most particulate systems contain many particles, and thus many equations have to solved at the same time.

The problem is further exacerbated when particles interact with each other, as these interactions need to be resolved on a particle-particle pair basis - so a naive implementation would imply a computational cost of N^2, where N represents the number of particles in the system.

During this lecture a short background will be given into DEM, and the reasons for applying it. Then, the two most important deterministic interaction models will be discussed: the soft-sphere model and the hard-sphere model.

Soft-sphere model

In the soft-sphere model, the deformation of the particles during their contact is approximated, and a resulting force is determined based on this deformation. This force can have a normal and a tangential component, where the normal direction is taken in the direction aligned with the two particle centers. The tangential component is perpendicular to this normal. In the soft-sphere model, more than two particles can interact, and the time of the interaction is actually resolved.

The simplest model for this is the fully elastic model, first proposed by Hertz. In the elastic model, the relative velocity between the particles before colliding is the same as the relative velocity after the collision. When the collision is oblique, the resulting force has a normal and a tangential component, as discussed in Mindlin and Deresiewicz (1953).
There are many more realistic interaction models as well, accounting for the plastic behaviour, such as in Thornton and Ning (1998) and visco-elastic behaviour, such as reviewed by Kruggel-Emden et al. (2008).
In the soft-sphere model, the governing equations are solved with a very small but fixed time-step. The magnitude of the time-step is limited by the stiffness of the material of the particles. Each full particle interaction (from first contact, to maximum deformation, back to detachment) needs to be resolved by a large number of integration time-steps, typically 30 - 80. When particles are of a stiff material, this total interaction time is typically very short, and thus the integration time-step has to be very small.

Hard-sphere model

In the hard-sphere model, the overall conservation of energy and momentum are applied to the pair of interacting particles, as in Hopkins and Louge (1991). This relates the pre-collision state to the post-collision state. Coefficients of restitution and a coefficient of friction is introduced to account for the inelastic nature of the collision and the Coulomb friction, respectively.

The hard-sphere model concept can only be applied to particles just before they collide, *i.e.* particles which are "just touching". Therefore, an algorithm will need to find the collision time for each pair of particles in the system, and update the particles positions to that time, before applying the conservation principles. Therefore, this is commonly referred to as "event-driven"; the algorithm is driven by the events of collisions, and the resulting time-step varies accordingly. It will be shown that the hard-sphere model is only for binary and instantaneous collisions.

During the lecture, attention will be given to the coupling with the fluid phase, where the so-called "Particle-in-Cell" method of Crowe et al. (1977) is typically applied. The lecture will also discuss a few applications and examples.

References

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