

Simulating convex polyhedral particles utilizing the discrete element method on GPU

Eva Siegmann*, Johannes Khinast^{◦*} and Gundolf Haase[†]

* Research Center Pharmaceutical Engineering GmbH, Inffeldgasse 13, Graz, Austria
e-mail: eva.siegmann@rcpe.at

◦ Institute for Process and Particle Engineering, Graz University of Technology, Inffeldg. 13, Graz, Austria

† Institute for Mathematics and Scientific Computing, Karl-Franzens-University, Heinrichstr.36, Graz, Austria

ABSTRACT

Simulations of granular flows are an effective tool to gain a deeper understanding and subsequently, optimization of processes such as fluidized beds, mixing, powder transport, etc. The discrete element method (DEM) allows simulating these kinds of processes. Each particle is treated individually and its motion is described by Newton's equation of motion. A soft-sphere approach is used, where colliding particles are allowed to slightly overlap. This overlap results in a repulsive force.

The particle shape plays a crucial role in modelling the process as realistically as possible. There are several approaches for modelling the shapes of more complex particles. The multisphere approach clusters several spheres to one rigid particle [1]. This approach is very flexible and can describe various shapes. Biconvex tablets can be represented as the overlap of three spheres. Superquadrics represent many shapes, such as ellipsoids, cylinder- and box-like particles [2]. To increase the accuracy, particles can be modelled as convex polyhedrons [3]. This approach allows simulating sharply-edged non-spherical particles. Although it is computationally expensive, it is the only way to model complex shapes realistically.

Where the collision of spheres is easy to handle more complex shapes are challenging. This work shows an accurate contact algorithm for arbitrarily shaped convex polyhedrons. The algorithm has been implemented in the GPU based DEM software XPS, allowing simulation of a very large number of particles [4].

REFERENCES

- [1] **Ketterhagen W.** Modeling the motion and orientation of various pharmaceutical tablet shapes in a film coating pan using DEM. *International Journal of Pharmaceutics, Volume 409, Issues 1-2*. May 2011, S. 137-149.
- [2] **Podlozhnyuk A., Pirker S., Kloss C.** Efficient implementation of superquadric particles in Discrete Element Method within an open-source framework. *Computational Particle Mechanics*. 2016, S. 1-18.
- [3] **Govender N., Wilke D.N., Kok S., Els R.** Development of a convex polyhedral discrete element simulation framework for NVIDIA Kepler based GPUs. *Journal of Computational and Applied Mathematics, Volume 270*. November 2014, S. 386-400.
- [4] **Jajcevic D., Siegmann E., Radeke C., Khinast J.** Large-scale CFD-DEM simulations of fluidized granular systems. *Chemical Engineering Science, Volume 98*. 2013, S. 298-310.