# A contact detection method between two convex super-quadric particles based on an Interior Point algorithm in the Discrete Element Method

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## ABSTRACT

Particle shape approximation is a challenging task in the Discrete Element Method (DEM) simulations. Spheres are easy to handle in a DEM-code and thus remain popular in particle representation because of their computational efficiency. Spherical particles behave differently than complex shaped bodies even on the single grain level. The most problematic tasks in non-spherical DEM simulations are the shape construction, the contact detection and the contact force calculation. Convex super-quadric (super-ellipsoidal) particles demonstrate an excellent trade-off between shape flexibility and speed of calculations in DEM[1]. Changing the set of parameters leads to various shapes like tablets, blocks, cylinders and others with rounded edges.

Contact detection between two super-quadrics is generally possible by solving a system of non-linear equations using the geometric condition that the line of minimal distance is orthogonal to the both surfaces and hence aligned with the normal vectors. These equations are the Karush-Kuhn-Tucker (KKT) conditions [2][3] of the following minimal distance problem (MDP):

$$\min\|\boldsymbol{x}_1 - \boldsymbol{x}_2\|$$
$$\text{s.t. } f_1(\boldsymbol{x}_1) = 0, f_2(\boldsymbol{x}_2) = 0,$$

where $f_1(\boldsymbol{x}_1)$and $f_2(\boldsymbol{x}_2)$ are the shape functions of the two interacting super-quadrics. The KKT conditions give necessary and sufficient conditions for solving of the MDP. However, above mentioned minimal distance problem is non-convex and the iterative procedure can get stuck or even diverge. Without loss of generality the MDP can reformulated using slack variables (an Interior Point Method):

$$\min\|\boldsymbol{x}_1 - \boldsymbol{x}_2\|$$
$$\text{s.t. } f_1(\boldsymbol{x}_1) + s_1^2 = 0, f_2(\boldsymbol{x}_2) + s_2^2 = 0.$$

Instead of adding the barrier term to the objective function $\min\|\boldsymbol{x}_1 - \boldsymbol{x}_2\|$ in this work we change the slack variables $s_1, s_2$ by its squares as shown above. The KKT system is solved by Newton's method coupled with GMRES linear system solver[4] as the Jacobian matrix is usually ill-conditioned. The main advantage of this approach that it requires only matrix-vector products, that can be approximated by taking difference of the non-linear function [5].

Following [6] we suggest to complete above mentioned approach by applying homothetical shrinking of particles, solving the MDP problem for shrinked particles and reconstructing the overlap by inversed homothety.

We describe the method that demonstrate robust convergence properties, high accuracy in terms of overlap distance and contact detection and show its implementation to a LIGGGHTS®[7] DEM code.

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