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Hopper flow of irregularly shaped particles (non-convex polyhedra): GPU-based DEM simulation and experimental validation

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HIGHLIGHTS

- A new GPU based contact method to handle both convex and non-convex polyhedra is presented.
- GPU based DEM is validated against experiment which tests the stability and accuracy of the contact method and GPU implementation.
- Stable archs are demonstrated for non-convex particles highlighting the importance of interlocking due to shape.
- Flexibility our implementaion is shown with simulations of up to one million non-convex particles as well as chain-linked particles.

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ABSTRACT

Numerous practical applications of the Discrete Element Method (DEM) require a flexible description of particles that can account for irregular and non-convex particle shape features. Capturing the particle non-convexity is important since it allows to model the physical interlocking when the particles are in contact. To that end, the most flexible approach to capture the particle shape is via a polyhedron, which provides a faceted representation of any shape, albeit at a significant computational cost. In this study we present a decomposition approach to modeling non-convex polyhedral particles as an extension of an existing open source convex polyhedral discrete element code, BlazeDEM-GPU, which computes using general purpose graphical processing units (GPGPUs). Although the principle of decomposition of non-convex particles into convex particles is not new, its application by the discrete element modeling community has been rather limited. The non-convex extension of BlazeDEM-GPU was validated using a hopper flow experiment with identical convex and identical non-convex 3D printed particles. The experiment was designed around two sensitive flow points, with the convex particles following the intermittent flow and the non-convex particles forming stable arches. It was demonstrated that the DEM simulations can be applied to reproduce both the convex and the non-convex flow behavior using the same parameter set. This study is a significant step towards general computing of non-convex particles for industrial-scale applications using the GPGPUs.

1. Introduction

In nature and in industrial processes, particles have various shapes, as depicted Fig. 1(a)–(d). A key ingredient in a DEM simulation is abstracting complex particles into shapes suitable for computation. Abstractions involve simple spheres, convex polyhedra, non-convex polyhedra and even non-convex large aspect ratio shapes, often resulting in entangled media. Some two-dimensional abstractions are depicted in Fig. 2(a)–(d). Spherical particles can be representative of silica gel and ceramic granules in chemical processing or peas in the food industry, while salt and sugar crystals can be sufficiently approximated by convex polyhedral-shaped particles. Crystalline powders, crushed gravel and cement particles can be represented by non-convex polyhedra, while entangled media contain rigid staples, flexible woven fabrics and particles formed during the granulation process.

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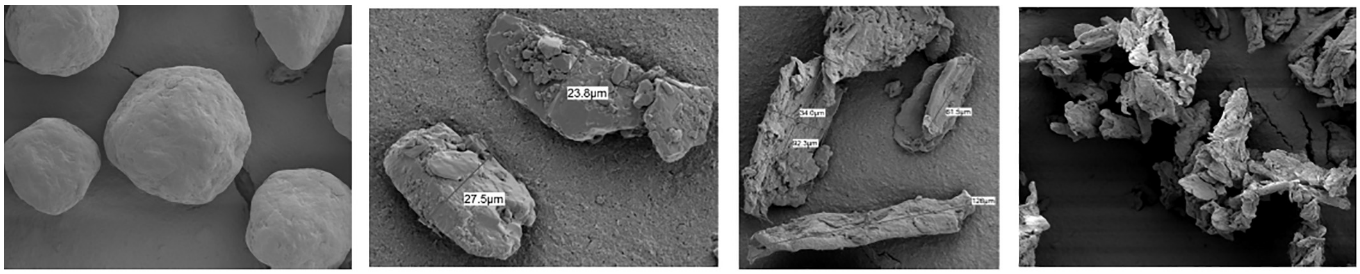

Fig. 1. Four examples of typical particles shapes for powders created by (a) spray-drying, (b, c) crystallization and (d) dry granulation that could be approximated by spherical, convex polyhedral, non-convex polyhedral and entangled non-convex polyhedral representations.

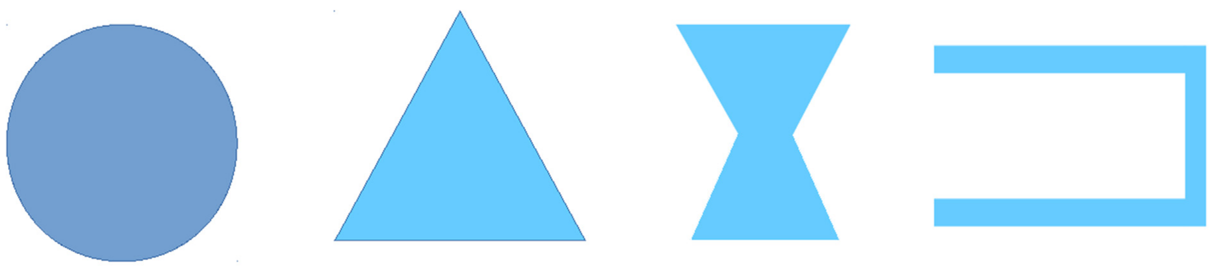

Fig. 2. Actual particle shapes abstracted as (a) spheroidal, (b) convex polyhedra, (c) non-convex polyhedra and (d) entangled non-convex polyhedra.

However, the geometrical abstraction of an actual particle is not the only consideration with regard to the DEM simulations. The computational cost plays an important role in terms of selecting the shape abstraction. In addition, many simulation software codes can only perform particular shape abstractions. The DEM shapes are mainly limited to spherical particles or smoothed polyhedral particles, with spheres or cylinders used for geometric features modeling. A common technique to model non-convex particles is the multi-sphere approach, in which particle shapes lack angularity (often a critical particle property in many applications) (Cleary, 2010; Lu et al., 2015; Windows-Yule et al., 2016). Moreover, flat surfaces are approximated by spherical packing, resulting in artificial surface roughness effects. Triangulation of particle surfaces aims to address some of the clumped sphere shortcomings (Fleissner et al., 2007; Smeets et al., 2015). However, both approaches involve a significant computational burden, which limits the number of particles that can realistically be considered. Consequently, the number of large-scale non-convex particles in simulations is limited. In general, there have been few particle-shape studies in large-scale discrete element simulations despite their well-established industrial importance (Cleary, 2010; Lu et al., 2015; Windows-Yule et al., 2016).

Large-scale industrial discrete element simulations can often only afford to abstract particle shapes as spheres or multi-spheres with few particles (Lu et al., 2015; Rougier et al., 2004; Kruggel-Emden et al., 2008; Shi et al., 2015). Utilizing graphics processing units (GPUs) in the DEM may speed up computational times and allows more complex particle shapes to be used in large-scale industrial simulations. Recently, it has been demonstrated that convex polyhedral shape abstractions, which used to require CPU computing architectures (Lu et al., 2015; Nezami et al., 2004; Boon et al., 2012; Hopkins, 2014; Podlozhnyuk et al., 2017; Rakotonirina et al., 2017), can efficiently be included in large scale industrial simulations using GPUs (Govender et al., 2014, 2015, 2018). This study extends the shape abstraction on the GPU architecture to include non-convex particle shapes and builds on the limited non-convex or concave particle shape DEM simulations that have been conducted on CPU architectures (Smeets et al., 2015; Rakotonirina et al., 2017; Matuttis and Chen, 2014; Lim et al., 2014; Williams and Connor, 1999; Nye et al., 2014; Yang et al., 2016; Gravish and Goldman, 2016). The initial non-convex/concave particle shapes were limited to two-dimensional abstractions, e.g., in the work of Lim et al. (2014), Yang et al. (2016), and Alonso-Marroquín (2008). This was extended to three-dimensional smooth abstractions, as demonstrated by Lim et al. (2014), which requires non-uniform rational b-spline (NURBS) surfaces to represent the particles and a contact grid to resolve contact. Fleissner et al. (2007) extended non-convex abstractions to include faceted bodies that can be in contact with spherical particles by conducting a surface triangulation of the faceted bodies. Smeets et al. (2015) generalized this approach by considering non-convex abstractions of particles and applying a surface triangulation to non-convex particles which allowed them to simulate up to 3000 non-convex particles. Recently, Rakotonirina et al. (2017) rekindled the well-known convex decomposition proposed by Nye et al. (2014), Bernard (1981), and Bajaj and Dey (1992) as a strategy to extend standard convex polyhedral contact resolution in order to resolve non-convex polyhedral contact using CPU architectures with MPI for 250 non-convex particles.

Following a convex decomposition approach, this study extends the convex polyhedral DEM code, BlazeDEM-GPU, to handle non-convex polyhedral-shaped particles on a GPU architecture. Our extension of BlazeDEM-GPU towards non-convex polyhedral shaped particles is validated against a carefully constructed experimental hopper discharge setup using monodispersed 3D printed particles. In addition, we demonstrate that we can compute a million non-convex polyhedral-shaped particles robustly and accurately within a realistic time frame due to the efficiency of our convex contact and decomposition implementation on the GPU.