3D Simulation of Packing of Heterogeneous Ellipsoidal Particles using Discrete Element Method

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ABSTRACT
Soil liquefaction, the phenomenon by which water-saturated soil temporarily loses strength due to dynamical loadings such as in earthquakes, can have dramatic consequences, e.g. collapse of entire buildings or destruction of dams and retaining structures. This paper deals with the modeling and simulation of dense packing processes for families of ellipsoidal particles of high aspect ratio and high volume ratio. The objective is to construct grain assemblies suitable to the numerical simulation of liquefaction Current simulations of these phenomena by the Discrete Element method are usually performed in terms of spherical particles. However, such a simple model for the description of the particles usually fails to provide accurate predictions of the behavior of actual grains of sand, one of the reasons being that contact forces and moments are incorrectly evaluated. The packing process consists in randomly dropping ellipsoids in a container and in applying unidirectional vibrations to the container to achieve dense packing. The process is repeated until a desired height is achieved and particles rest in a stable position. Interactions between particles are simulated in this work using the Discrete Element Method. Numerical examples for various distributions of aspect ratios and volume ratios will be presented in order to demonstrate the efficiency of the proposed approach.

RÉSUMÉ
L'article porte sur la modélisation et la simulation de procédés d'entassement dense pour des familles de particules ellipsoïdales à rapport de forme et rapport volumique élevés. Le principal objectif est de construire des assemblages de grains qui soient appropriés à la simulation du phénomène de liquéfaction des sols. Ce phénomène, par lequel un sol saturé d'eau perd temporairement sa résistance sous l'effet d'un chargement dynamique, comme par exemple lors d'un tremblement de terre, peut avoir des conséquences catastrophiques, e.g. l'effondrement de bâtiments ou la destruction de barrages ou de structures de soutènement. Aujourd'hui, les simulations de ces phénomènes par la méthode des éléments discrets sont souvent basées sur l'utilisation de particules sphériques. Cependant, ce simple modèle pour la description des particules ne permet pas de correctement prédire le comportement de véritables grains de sable, l'une des raisons étant que les forces et moments de contact entre particules sont incorrectement évalués. Le procédé d'entassement consiste ici à déposer de manière aléatoire des ellipsoïdes dans un contenant et à appliquer des vibrations unidirectionnelles au contenant pour obtenir un entassement dense. Le procédé est répété jusqu'à ce que l'on obtienne la hauteur désirée et que toutes les particules aient atteintes une position stable. Les interactions entre particules sont simulées ici par la méthode des éléments discrets. Des exemples numériques pour différentes distributions de rapports de forme et volumique seront présentés afin de démontrer l'efficacité de la méthode proposée.

1 INTRODUCTION

Packing of particles is the process by which particles are assembled together in a given container. It is in general a very computationally-intensive process as it requires information about all possible interactions between particles. Many applications in science and engineering need a better understanding of the physics of particle assemblies, e.g. packing of rice grains, medicinal powders, ceramic powders, sand, granular materials, etc. Objectives of packing studies are, for instance, to evaluate the mechanical properties of composite materials (Zhuang et al. 2017), to obtain optimal packing conditions in cement (Stroeven and He, 2013, Xu and Chen 2012), to model powder-based structures (Zhou et al. 2009), to name a few. A general objective when studying packing processes is to find the type of particle shape and packing method that will produce the densest arrangement. Another objective is the simulation of physical phenomena involving real particles for which the modeling of their mechanical behavior is crucial, e.g. the fluid flow through porous media such as sands, gravels, or sediments. In this case, it is important that the packing method be capable of reproducing specific properties (density, porosity, granular structures, size distribution, etc.) of actual grain samples. This has led to the development of numerical approaches to model the packing of particles.

The paper is organized as follows: in Section 2, we review some notions of packing methods and list a number of approaches that have been proposed in the literature in order to motivate our work. We discuss in Section 3 some of the packing methods that are more suitable for ellipsoidal particles. We then briefly review the Discrete Element method in Section 4, describe the methodology of our approach in Section 5, and present preliminary results in Section 6.

2 PACKING METHODS

In order to assess the quality of packing methods with respect to actual samples, several quantities are usually considered. A common quantity is the *packing fraction* ρ, also referred to as the *packing density,* which determines the volume of fluid that fills the void between particles. It is simply calculated by taking the ratio of volume of the particles and that of the container. A similar quantity is the *porosity* μ defined as $\mu = 1 - \rho$. In general, the packing density depends on the *particle size distribution* (PSD), particle shape, material properties of particle, relative size of the container, and packing method (Zhou et al. 2011, Baram and Lind 2012, Delaney et al. 2005, Williams and Philipse 2003). Depending on the value of the packing density, a given packing can be referred to as loose or dense.

In the case of mono-sized spheres, the density of a dense packing typically ranges from 0.610 to 0.665 and that of a loose packing from 0.580 to 0.606 (German 1989). In the case of disks, it has theoretically been shown that the maximal value of the packing density is $\pi/\sqrt{12} \approx 0.9$ (Pach and Agarwal 2011).

In the case of ellipses, the packing density is measured with respect to their aspect ratios. As the aspect ratio of the particles is increased, the packing density increases up to a maximum and then decreases (Zhou et al. 2011, Baram and Lind 2012, Delaney et al. 2005, Gan et al. 2016 I, Donev et al. 2004). However, if the ellipses are prevented from rotating during the packing process, the density remains almost constant with increasing aspect ratio and then decreases slowly (Delaney et al. 2005). The maximum density has been attained, in the case of oblate spheroids and prolate spheroids, for aspect ratios of 0.6 and 1.8, respectively (Zhou et al. 2011), and similarly, for aspect ratios of $1/\sqrt{3}$ and $\sqrt{3}$ (Donev et al. 2004). Note, however, that another study (Sherwood 1997) provided a maximum packing density at values of the aspect ratios equal to 0.7 and 1.4. In 2D, in the case of particles with elliptical shape, the maximum density of 0.895 was reached for an aspect ratio equal to 0.664 (Delaney et al. 2005).

For general non-spherical particles, the shape of particles is usually measured in terms of the *sphericity*, which is the measure of how closely the shape of an object approaches that of a mathematically perfect sphere. It is defined as the ratio of the surface area of a spherical particle to that of a non-spherical particle when their volumes are identical. For example, it was reported that changing from spherical to non-spherical particles provided a maximal packing density at sphericity 0.83 (Zhou et al. 2011). The effect of sphericity on porosity is different in loose and dense packing. In a loose packing, the porosity decreases by increasing the sphericity. However, in dense packing, the porosity will increase after reaching a minimum when increasing the sphericity. Moreover, different trends were found for the sphericity of cylinders and disks. Consequently, the relationship between these two parameters depends on the packing method and the shape of particles (Zou and Yu 1996).

Another measure for assessing packing algorithms is the so-called *coordination number* (CN), which is the number of particles in contact with a given particle. This parameter also provides a means to consider whether the packing is ordered or disordered. The coordination number and the packing density are not necessarily correlated. Indeed, the two parameters are related in the case of oblate spheroids but are not in the case of prolate spheroids (Zhou et al. 2011).

The packing structure can also be described in terms of the *radial distribution function* (RDF), which shows the probability of a given distance between the centers of particles. In other words, it measures the probability of finding a particle between the distances r and $r + \Delta r$ from the center of a given particle. The RDF for spheres is given by (Yang et al. 2003, Zhou et al. 2011, Gan et al. 2016 I):

$$g(r) = \frac{N(r)}{4\pi r^2 \Delta\, r\, \rho_0}$$

where $N(r)$ is the number of particles whose centers lay between r and $r + \Delta r$ and ρ_0 is the number of particles per unit volume calculated as

$$\rho_0 = \frac{6\epsilon_s}{\pi d^3}$$

Here ϵ_s is the packing density and d is the particle size (Zhou et al. 2011, Gan et al. 2016 I). For spherical particles, Δr is set equal to $\Delta\, r = 0.02d$, since the average of the RDF is obtained at this value (Yang et al. 2003, Gan et al. 2016 I, Zhang et al. 2001). For ellipsoidal particles, it is set to $\Delta\, r = 0.02d$, where $d = 2(abc)^{1/3}$ is a measure of the size of the particle, with a, b, and c the three semi-axes of the ellipsoids (Zhou et al. 2011, Gan et al. 2016 I).

It is also worth mentioning that the material properties of particles can strongly affect the resulting packing structures. For instance, the packing density increases with respect to both the sliding and rolling friction coefficients and the Young modulus of ellipsoidal particles (Zhou et al. 2011). Similarly, for fine spherical particles, the porosity decreases by increasing the sliding and rolling friction coefficient and the Hamaker constant (Yang et al. 2003). The sliding and rolling friction coefficients are related to the forces acting on the surface of the particles while the Hamaker constant is related to the body forces, e.g. Van der Waals forces, that describe the particle interactions. Finally, the size of the container may also affect the packing density. The effect of the container wall decreases as the size increases. Therefore, an approximate linear relationship with a negative slope is found between the size of the container and the packing density (Zhou et al. 2011). The height at which particles are dropped in the container can also affect the packing density in the case of spherical particles. The packing density increases when the dropping height increases up to 150 cm and then remains unaffected (Zhang et al. 2001).

In general, packing algorithms are categorized as either regular or random packing methods, whether the particles are deposited regularly or randomly. Most packing methods have been introduced for circular and spherical

particles, even though some of them can be generalized for other particle shapes. We provide below a brief description of existing packing methods:

- **Random sequential addition (or adsorption) (RSA):** Particles are placed randomly one by one. If a newly positioned particle overlaps another one, it is removed, otherwise it is kept permanently. The denser the packing becomes; the more probable particles overlap. The method is usually called adsorption in 2D (Evans 1993) and addition in 3D (Sherwood 1997). It has been used to pack spheres (Talbot et al. 1991, Zhou et al. 2009, Coelho et al. 1997) and ellipsoids (Sherwood 1997, Anoukou et al. 2018). The RSA method is less complex than other methods, which makes it attractive (Ghossein et al. 2013), but also exhibits low efficiency (Recarey et al. 2019). Moreover, the method does not necessarily describe a realistic physical phenomenon (Sherwood 1997).
- **Lubachevsky and Stillinger (LS) Algorithm:** In this method, particles are generated randomly with null volume. A random velocity is assigned to each particle and the volume is gradually expanded until collision (Lubachevsky et al. 1991). It is reported that the LS algorithm generates not only denser packing but is also more efficient than RSA (Ghossein et al. 2013).
- **Advancing Front Algorithm**: In this method, two or three particles are positioned at first in the container. The next particle is then deposited in front of the pre-existing particles, in such a way that there is no overlap with them. The position is rejected as long as there is no overlap with the other particles (Feng et al. 2002, Feng et al. 2003, Benabbou et al. 2010, Recarey et al. 2019). In case of using random size distribution, the disadvantage of the method lies in the fact that the edge of the container is not filled up with particles (Bagi 2005).
- **Dropping and Rolling (DR) Algorithm**: This algorithm is a type of RSA. Each particle is dropped on the floor of the container or on pre-existing particles. The particle is rolled until it gets into a stable position and touches three particles (if it is possible) or the floor (Shi and Zhang 2006, Zhou et al. 2009). The disadvantages of the DR algorithm are inefficiency for small particles and the fact that is uses periodic boundary condition.
- **Optimized Dropping and Rolling (ODR) Algorithm**, no boundary condition is used. Moreover, the method is twenty times faster than DR as a maximum number of rejections is set to stop the algorithm (Hitti and Bernacki 2013).
- **Sedimentation Packing Algorithm:** The method is similar to the DR algorithm. Spheres in the first layer are positioned randomly and other layers are dropped under the influence of gravity on the first layer. Then, the overlap is illuminated through several iterations that consist in sorting, moving, and rotating the spheres until they reach a stable position (Nolan and Kavanagh 1992).
- **Compression Algorithm:** The method is used for packing spheres (or circles) with high efficiency. The packing is randomly initialized with spheres of various sizes. The following stage in order to densify the packing includes two steps: (1) compressing step and (2) refilling step. The two steps are repeated one after the other until it becomes impossible to run either one (Han et al. 2005).
- **Triangulation Based Approach:** The domain is first partitioned into random triangles. Circular particles are then inscribed inside the triangles. Additional particles are positioned at the nodes (non-overlapping) to densify the packing (Cui and O'Sullivan 2003). The method can also be used with tetrahedra and spheres. The coordination number and packing density of this method are lower than those obtained from the sedimentation and advancing front algorithms. However, the method is simpler and more efficient (Bagi 2005).
- **Poured-packing Procedure**: In this method, particles are dropped from a specific height into a cylindrical container. In order to limit the number of collisions between particles, a small velocity is applied to each particle (German 1989).
- **Inwards Packing Method**: The particles are first deposited as a chain with no overlap along the perimeter of the domain. After filling up the edges, a new particle is positioned in contact with two other particles inside. When it is not possible to add another particle with the desired random size distribution, smaller particles fill the gap between particles (Bagi 2005). The method produces high coordination numbers and packing densities. However, its disadvantage lies in the fact that the porosity cannot be controlled by users.
- **Voronoi Tessellation Packing or Stienen Model**: The packing is initialized using the RSA to randomly position disks. A Voronoi tessellation is then used to create a polygon around each disk. The center of each disk is moved to the center of the largest inscribed circle the polygon and the diameter of the disk is let to increase while avoiding overlaps. This approach generates a random dense packing (Hinrichsen et al. 1990).
- **Jodrey-Tory (JT) Algorithm:** In this algorithm, a specific number of points are generated and positioned randomly. Each point is identified as the center of a sphere. Each sphere is then associated with an inner and an outer diameter. The inner diameter is evaluated based on the minimum possible distance of the centers of two spheres without overlap. Through an iterative approach, the outer diameter is decreased while spheres are displaced to eliminate overlaps. This algorithm generates a dense packing (Jodrey and Tory 1985).
- **Force-Biased (FB) Algorithm:** The algorithm is initialized in the same way as the JT algorithm. Rather than applying an iterative algorithm to determine a dense packing, a force is applied to each particle, which leads to a slow restructuring of the grain assembly. The force is related to the overlapping area of the particles and the resultant displacement vector (Mościński et al. 1989). The algorithm leads to a denser packing than the JT algorithm.

- **Zinchenko Algorithm**: This approach is based on a contact network. Random spheres are initially positioned in the domain. Then, each sphere is allowed to grow until it comes into contact with at least another sphere. At that point, the sphere freezes and stops growing (Zinchenko 1994).
- **Geometric Packing:** The goal of this method is to maximize the packing density. In order to do so, small particles fill the voids between the assembled particles using a discrete or continuous distribution of particles (Brouwers 2006).
- **90° Rotation Algorithm:** In this method, a loosely packed layer of particles is randomly created and kept fixed in the domain. A second layer, which is identical to the first layer but rotated by an angle of 90°, is placed on top of the first layer. The particles in the second layer are then allowed to move and fill the gaps within the first layer. New layers are added in the same manner until a desired height is reached (Chekired and Roubtsova 2014).
- **Adaptive Shrinking Cell (ASC) Algorithm**: The goal of the algorithm is to generate a dense packing of non-spherical particles. The problem is formulated as an optimization problem subjected to periodic boundary conditions. The method is in general more efficient than the LS algorithm (Torquato and Jiao 2009, Torquato and Jiao 2010).

3 PACKING OF ELLIPSOIDAL PARTICLES

Most algorithms have traditionally focused on the packing of spherical particles. More recently, algorithms have been considered for ellipsoidal particles. Ellipsoids are interesting due to their capability to represent a wide range of shapes, from elongated geometries to spheres. One motivation for studying ellipsoidal particles is to investigate the effect of particle shape on the packing properties, when compared to spherical particles (Stroeven and He 2013, Zou and Yu 1996 , Donev et al. 2004, Zhou et al. 2011, Zhou et al. 2013, Gan et al. 2016 I, Gan et al. 2016 II).

Modified versions of the aforementioned packing methods have been extended to the case of ellipsoidal particles. For instance, when using the RSA, the position of randomly initialized ellipsoids is kept fixed if it lies inside the container and non-overlapping constraints are met to ensure no overlap with other particles (Sherwood 1997, Xu and Chen 2012). In the poured-packing procedure, ellipsoidal particles are dropped with an initial velocity from a predefined height to fill a cylindrical container layer-by-layer (Zhou 2011). Voronoi tessellation can be used for ellipsoidal particles to generate dense packing. The objective is to find the densest packing by minimizing the Voronoi cell volume (Schaller et al. 2016). In yet another example, ellipsoids, generated with a random size and orientation, are moved to the bottom of a container until they enter into contact with other ellipsoids. Once the ellipsoids are assembled, an initial velocity with random direction and magnitude is applied to the particles in order to densify the packing (Lee et al. 2003). The objective in the advancing front algorithm for ellipses is to pack, without overlap, a new ellipse in contact with existing ellipses. The center of the new ellipse is actually obtained by sliding the ellipse in a pure translation along each of the two existing ellipses on the active front and by computing the intersection points between the two loci (Feng et al. 2002). Nevertheless, there are some techniques that have been specifically developed to pack ellipsoidal and elliptical particles. However, most methods were designed for 2D problems:

- **Optimal Packing of Ellipses in a Container:** This class of methods are based on the formulation of an optimization problem. As an example, for a circular container, the goal can be to optimally position ellipses of different sizes into a circle with a minimal radius. An optimization problem is then set up in order to minimize both the radius of the circular container and the distance between non overlapping ellipses (Kampas et al. 2016). In the case of a square container, a model problem consists in packing two ellipses of same size while maximizing the packing density (Gensane and Honvault 2012). An extension to the previous problem is to place a maximum number of similar ellipses in a rectangle. This can be achieved by partitioning the rectangular domain and positioning the center of the ellipses at the nodes of the triangulation (Galiev and Lisafina 2013). In another example, the optimization problem consists in minimizing the apothem of a regular polygon (Kampas et al. 2019). For an ellipsoidal container, the optimization problem aims at minimizing the overlap between ellipsoids (Uhler and Wright 2013}.
- **Advancing Layer Algorithm (ALA):** In this method, an ellipse is constructed in terms of several inscribed circles. The first ellipse is positioned such it is in contact with the edges of the container. The other ellipses are then added so that there exists a contact between the inscribed circles associated with the ellipses. In other words, each ellipse is in contact with at least another ellipse (Ilin and Bernacki 2016).

Several methods have been proposed to simulate assemblies of particles. For instance, molecular dynamics (MD) simulations (Ghossein et al. 2013, Zhuang et al. 2017) allow one to calculate the thermodynamic and kinetic properties in order to study the elastic collision of particles. Other methods, such as Monte Carlo or the Discrete Element Method (DEM) have also been considered in (Abreu et al. 2003) and in (Zhou et al. 2011), respectively. A comparison between the DEM and the MD algorithms for ellipsoids has been carried out in (Zhou et al. 2011). DEM provides the information about all contact forces between particles, including gravity and torque, while in MD only elastic forces are considered. In addition, DEM simulates particles based on physical mechanisms while MD applies some treatments and assumptions which are not always physical. Moreover, DEM considers the energy dissipation coming from friction, collision, and rolling, while in MD these factors are not considered. In fact, the MD algorithm only minimizes the energy to achieve a stable pack of particles. Therefore, the DEM is more comprehensive and should provide more accurate results than the MD algorithm when modeling granular materials.

4 THE DISCRETE ELEMENT METHOD

The Discrete Element Method (DEM) was first proposed by Cundall and Strack (Cundall and Strack 1979), although it had been initially introduced in 1971 (Cundall 1971) to analyze rock mechanics problems. The method considers small displacements and rotations of the particles and identifies new contact between particles after each motion. The particles, which are assumed rigid, are allowed to overlap in order to account for deformation. Interactions between particles are accounted for in terms of contact forces. The Newton's second law and the force displacement law are used to model the motion of the particles. The position and velocity of the particles are updated based on the integration of Newton's second law using numerical methods such as the leap-frog integration scheme, the backward or forward finite difference methods, the Beeman's algorithm, or the Verlet integration scheme (Manne and Satyam 2015). The force-displacement relation is used at the contact points between particles to compute the resultant normal and tangential forces. DEM thus consists of five steps: particle initialization, collision detection, contact force calculation, application of the Newton's second law, and updating of the particle positions and velocities. The method can become computationally intensive when considering large assemblies of particles as above steps should be evaluated at each time step.

5 METHODOLOGY

Soil liquefaction is a phenomenon by which water-saturated soil temporarily loses its strength due to dynamical loadings, for example during earthquakes. It can have dramatic consequences, such as the collapse of buildings and the destruction of dams and retaining structures. The strength of the soil is roughly determined by the soil packing, and more specifically, by the contact forces between the individual grains. Hydro-Quebec has been developing a software, SiGran, to model the packing and fluid flow in water saturated soil samples, in order to improve their understanding of soil liquefaction near dams. The code was initially developed using spherical particles with rough surfaces to describe soil particles. The code has recently been upgraded with ellipsoidal particles by implementing the minimum distance algorithm for contact detection between ellipsoids. The packing process consists in randomly dropping layer of arbitrary size and shape of ellipsoids in a container, until a desired height is attained. Each layer is permitted to reach a stable state before the next layer is deposited. Interactions between particles are simulated in this work using the Discrete Element Method (DEM). Particles in DEM are usually represented as discs and spheres, in two-dimensional and three-dimensional problems, respectively. One obvious advantage of using such types of particles are that it is straightforward to find the contact points between pairs. Unfortunately, spheres are different from real soil particles in terms of shape, position of their centers of mass with respect to contact points, and hence, the manner by which one rotates around the other. Therefore, a recent trend is to consider particles with more complex shapes, such as ellipses or ellipsoids, polygons, superquadratics, collections of continuous circular segments, or clusters of spheres. However, using particles with complex shapes has the drawback that it becomes more difficult to detect contact points. Ellipsoidal particles not only have the advantage of simplicity compared to other shapes but also more closely match the shape of real grains than spheres. Another advantage of ellipsoids compared to spheres is that the normal contact forces induce a moment to the particles. This will in turn affect the rotation and resistance of particles and should better describe the behavior of actual grains. Detection of contact points between ellipses or ellipsoids is however more computationally demanding than with circular or spherical particles. In fact, if one uses an overlapping approach, the contact points and normal directions at those contact points are not unique. It follows that a variety of methods and algorithms, such as those in (Rothenburg and Bathurst 1992, Ting et al. 1993, Džiugys and Peters 2001, Mustoe and Miyata 2001), have been proposed and developed over the years in order to address these issues. Following a comparative study of these methods, we concluded that the minimum distance algorithm (Mustoe and Miyata 2001) is the most stable method for finding contact points between ellipsoids.

The code implementing the new packing algorithm is partially verified by reproducing the results of the old algorithm with those obtained with the new algorithm in the case of spheres. The resulting packing depends largely on the quality of the estimation of the contact points and of the planes normal to the contact. From a physical point of view, we also determine if assemblies of ellipsoids provide any new or more relevant macroscopic data when compared to those of spheres.

6 PRELIMINARY RESULTS

The algorithms added to the SiGran virtual laboratory extend the capabilities of the code to deal with more realistic simulations of granular materials. Moreover, the SiGran visualization capabilities help to access information that is very difficult, if not impossible, to obtain in actual laboratory experiments. Preliminary studies conducted with SiGran are described in (Roubtsova et al. 2011), (Chekired and Roubtsova 2014) and (Chekired and Roubtsova 2016). Upon implementation of the new algorithms for ellipsoidal particles into SiGran, we have conducted several numerical tests to assess the performance of the code. The first test dealt with the packing of particles of two different sizes interacting with each other under the action of gravity. An example is shown in Figure 1(a) that describes the relative particles and velocities of particles obtained with the packing method implemented in SiGran. The second test involved particles with three different sizes. In this example, one type of particles was much larger than the other two. The result is shown in Figure 1(b). We compared the void ratio in those two tests and concluded that the presence of particles of larger size tends to slightly increase the void ratio (0.86 vs. 0.84).

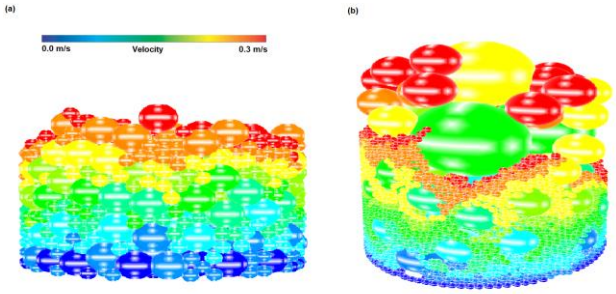

Figure 1. Relative positions and velocities with (a) two and (b) three different sizes of particles obtained with the packing method implemented in SiGran.

7 CONCLUSION

These algorithms will need to be carefully compared with respect to specific criteria (e.g. packing density and efficiency) that should be utilized according to the applications of interest. It appears that most of the algorithms were developed in order to accelerate the initialization of packing. However, more attention should be paid to whether speed up the cost on the initialization or not.

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