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REAL GRAIN SHAPE ANALYSIS: CHARACTERIZATION AND GENERATION OF REPRESENTATIVE VIRTUAL GRAINS. APPLICATION TO RAILWAY BALLAST.

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Abstract. Grain shape significantly influences the mechanical properties of granular media. In order to explore this effect and to simulate realistic material morphology, we designed a method which well characterizes real grains shape. Starting from a representation of the particle surfaces as a points cloud, this paper presents a method to generate a set of virtual grains that are morphologically representative of real ballast grains. The model relies on a statistical modelling of the ballast grain morphology based on a dimensionality reduction approach (Proper Orthogonal Decomposition) leading to an optimal and nearly exhaustive shape characterization by extracting a hierarchy of shape functions that fully describe the grain sample. We will show the efficiency of the both characterizing and generating methods and describe their advantages, as well as a future outlook

1 INTRODUCTION

Granular materials are widely used in different applications ranging from food industry to civil engineering. Therefore, a better understanding of the overall behaviour of these materials is pivotal to improve and control their performance. Numerous studies have been carried out and enriched over the last years, about the impact of particle size, shape and mineralogy on the mechanical behaviour of the granular media. As for shape properties, several experimental analyses as well as numerical studies using Discrete Element Methods (DEM) [1] have shown the significant influence of particle shape on the evolution of granular assemblies [2-6, 11-13, 16, 17, 24, 26]. Understanding this influence is then a topic of interest in this study.

For DEM simulations, representing particle shape is a real challenge. Most discrete element codes represent particles as discs (2D) or spheres (3D), because of implementation simplicity and computational efficiency. However, it has been proved that these simple geometries fail to reproduce realistic material behaviour for an individual grain, as well as for a granular assembly [7, 14, 20]. Other attempts have then been made to take into account complexity that falls roughly in two classes: 1) parametric model based on given geometric construction rules and 2) fitted model based on real grain shapes. Both approaches can be fulfilled with simple primitive (sphere, ellipsoid, plane, clumps...) or with more versatile geometric shape as polyhedron [8, 10]. Over the last decades, SNCF (French railway company) has chosen the second approach to simulate the behaviour of the ballast with DEM based on polyhedron shaped particles. Railway ballast is a granular layer formed by irregular rock grains of a centimetric size extracted from hard stone quarries by crushing ((BS EN 13450, 2003) [1]). Currently, virtual grains used in simulations are sets of nearly 1000 sampled grains that have been 3D digitalized and meshed.

In order to properly study the impact of the ballast shape on the mechanical behaviour with DEM, a generator of virtual grains is needed, apt to produce large sets of virtual grains that are representative of a limited set of real grain, and that also allows to reach an accurate characterization of the grain shape. In this paper, we propose a method to achieve these goals. In Section 2, the proposed approach of real ballast grain shape modelling as well as its validation are presented and analysed. Some illustrations are presented in Section 3.

2 REAL BALLAST GRAINS MODELLING

2.1 Global view

In the literature, generation methods were presented, such as Fourier-Shape-Descriptors [19, 22], and spherical-based random fields [9, 18, 29]. These approaches have given good results in terms of similarity of generated grains and real ones, but introduce shape functions that are imposed.

We present in this paper an innovative approach based on a dimensionality reduction method leading to an optimal and nearly exhaustive shape characterization of real grains.

By means of Proper Orthogonal Decomposition (POD) [15], we identify the optimal hierarchy of shape functions that describe the grain set. The main advantage of this approach is to reduce the number of needed shape functions to represent the grain shape with a quantitative controlled approximation (error based), such that we reduce the parametric space to the optimal one.

2.2 Pre-processing: Sample preparation

A database of 121 different ballast grains is provided by SNCF. Ballast materials in France are selected based on the European railway ballast specification. The grains are represented by point clouds obtained experimentally by 3D digitization (3D scan) of the particle surfaces, and form irregular polyhedrons of 4000 faces, and about 2000 vertices. Fig.1 shows some of these grains.

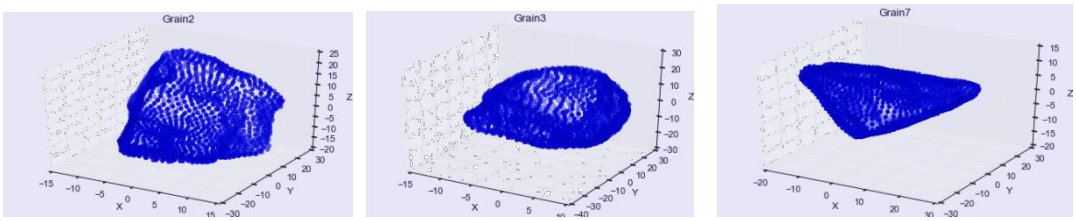
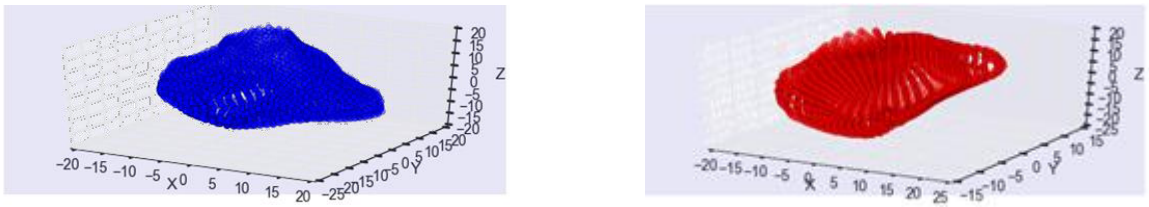


Figure 1 : Example of real ballast grains represented by dense point clouds - SNCF

The pre-processing is based on the following steps:

- ✓ Projection of the experimental points cloud on an imposed basis (B1) with constant angular step and N directions. Since the experimental point cloud are composed of many points (up to millions for finer digitalization) with random direction in a spherical frame, this step aims at reducing the number of point and having the same direction for each grain.
- ✓ Computation for all grains of volume, surface, inertia tensor, and mean radius.
- ✓ Centering grains and rotating vertices until the principal directions of the inertia tensor are parallel to the global coordinate axes, and interpolating (Fig.2)



(a) (b)

Figure 2: A grain of ballast: (a) Raw data (b) After projection and rotation

- ✓ Projection on a new basis (B2) with uniform density of number of direction by solid angle. Indeed, the previous basis, with constant angular step, lead to a high density of direction near the pole that can bias the statistic. This new basis with 500 directions is generated with a repulsion point iterative procedure. (Fig. 3)
- ✓ By concatenating all grains together, our set of experimental grain is then represented by a 500 x 121 matrix. Each column represents grain vertices distances along the 500 of the basis B2 (Fig.4). This matrix will be the input data of POD procedure.

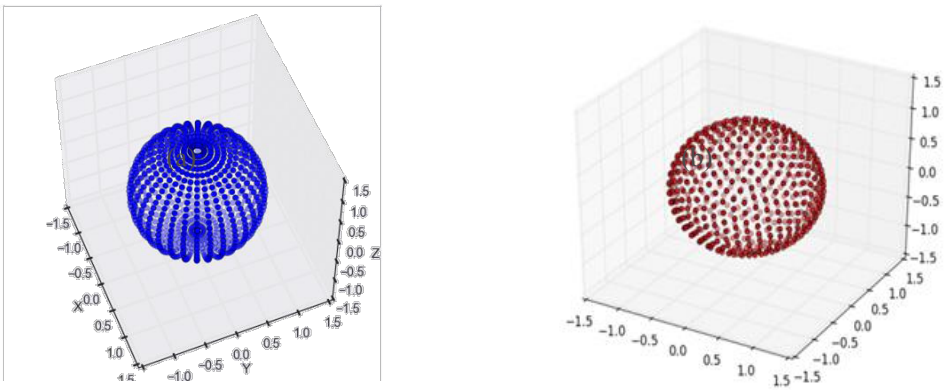


Figure 3: Basis with 500 direction: (a) basis B1 (b) basis B2

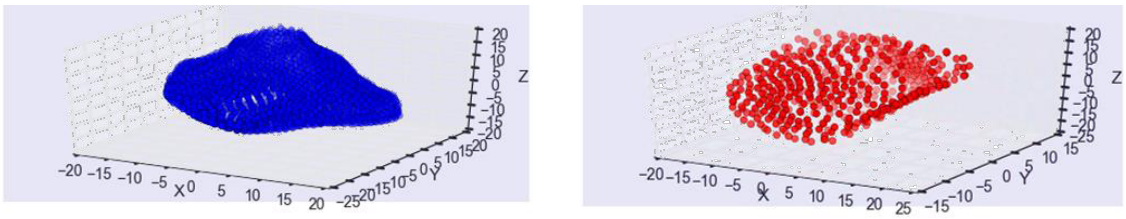


Figure 4: Interpolation on the generated basis with 500 directions and real grain

2.3 Grain characterization

A model reduction method, namely the Proper Orthogonal Decomposition or Principal Component Analysis (PCA) [27] is used. Starting from the data matrix of the Section 2.2, this multivariate statistical method aims at obtaining a compact representation of the data. It identifies an optimal and useful set of basic functions that allows to achieve a satisfactory approximation of the system.

This method serves two purposes, namely order reduction by projecting high-dimensional data into a lower-dimensional space and feature extraction by revealing relevant, but unexpected, structure hidden in the data. The first purpose allows to quantify the controlled approximation (error based), while choosing the dimension of the projection reduced space. The second purpose allows to characterize the shape features by associating them to POD outputs, i.e. basis functions (eigenmodes) and coefficients. Eigenmodes, or principal components, are the eigenvectors of the covariance matrix corresponding to original data, whereas coefficients are projection coordinates on the reduced space of projection. These two elements, in addition to eigenvalues of the covariance matrix are the three key elements of the method. For further explications of the method, see [15].

While applying POD on the data, a corresponding error ε is expressed in terms of the projection errors that are controlled in the construction of POD bases. In other words, it is defined as the deviation of the transformed data to the new space from the original data, normalized by the raw data and induced by the truncation of the POD basis. While POD error gives an indication of the magnitude of the "missing" information, the

energy of the system $e(k) = 1 - \varepsilon(k)$ represents the quantity of information captured by the k first POD basis vectors. (Fig. 5) shows the quantities of error/energy as a function of the dimension of the reduced space.

For zero error we have to keep all 121 modes. We see that with only 12 modes we represent 90% of the information and 99% of the information is represented with roughly 50 modes. With this precision, we have half-reduce our data.

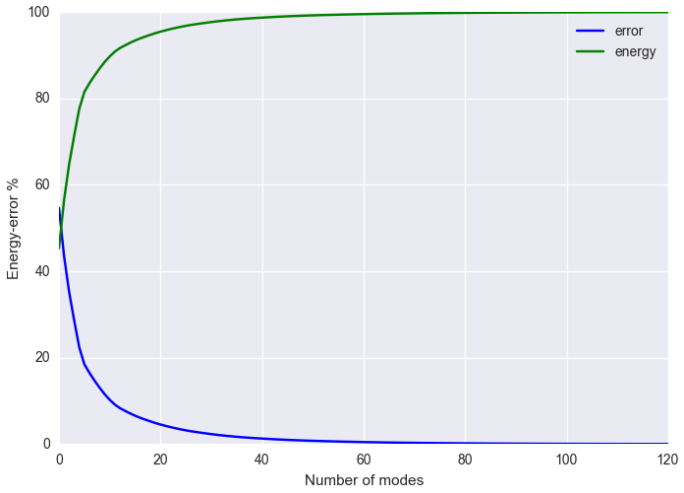


Figure 5: Error and energy quantification

As the accuracy of the grain approximation depends on the number of modes, it is important to check if the properties of grains (average radius, surface, volume) are sensitive to the number of modes. In (Fig.6), we compare those properties distributions for different error thresholds.

In order to quantify more precisely the comparisons, we perform Kolmogorov-Smirnov (KS) tests between original data surfaces/volumes/mean radius and reconstructed grains characteristics. The results are presented in Table 1.

Table 1: Values of Kolmogorov-Smirnov tests between original and reconstructed data S, V, Rm distributions

		KS Surfaces	KS Volumes	KS Rayons moyens
Error on shape	0.1%	0.999	0.997	0.947
	1%	0.999	0.997	0.879
	5%	0.999	0.997	0.785
	10%	0.997	0.984	0.465
	15%	0.984	0.879	0.223

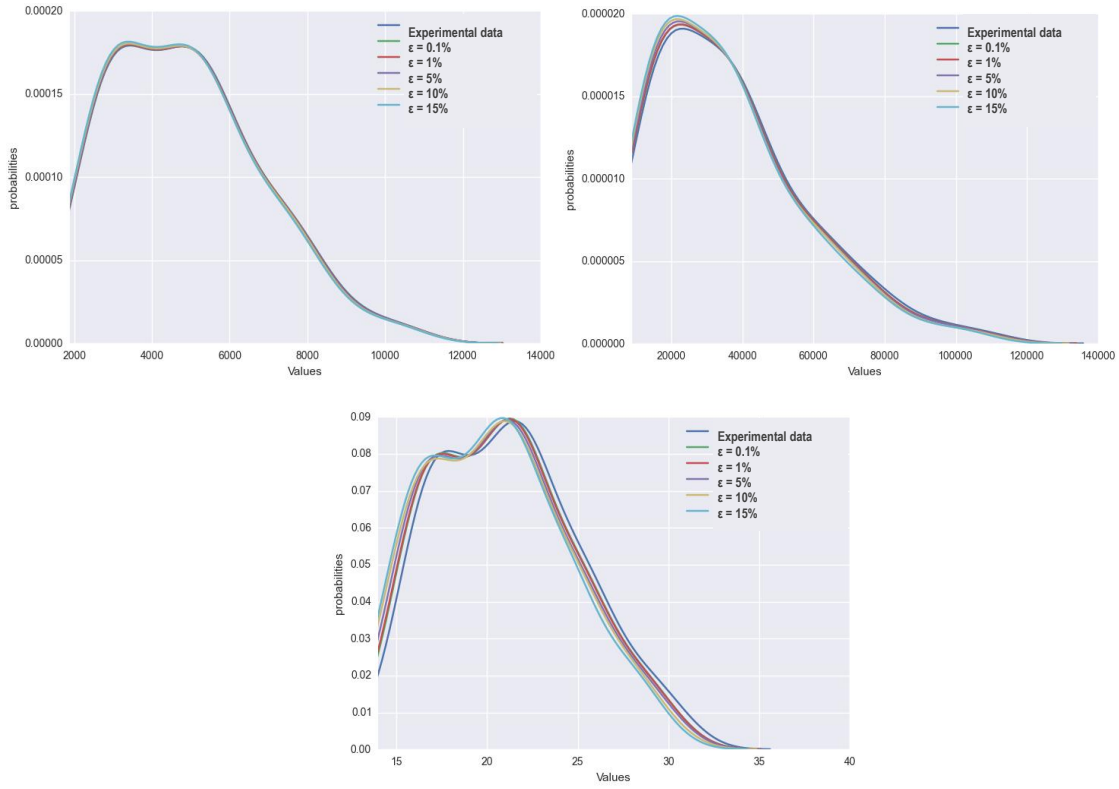


Figure 6: Reconstruction of the real grains for different error thresholds – Comparison of (a) Surfaces distributions (b) Volumes distributions (c) Mean radius distrbutions

We see that even with significant error (more than 10%) we have a very good shape approximation but with a much more reduced space.

Furthermore, by statistically identifying POD coefficients distributions, we can generate as many equivalent data as wanted. For a perfectly exhaustive shape characterization, we decide to keep all of the eigenmodes and therefore an error of 0% is made. The statistical analysis will concern the coefficients that are uncorrelated. (Fig. 7) shows statistical distributions of the first 8 coefficients as an example.

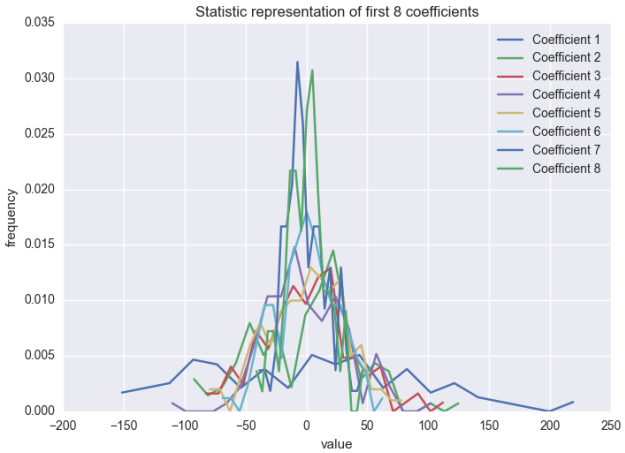


Figure 7: Statistic representation of the first 8 coefficients

The challenge is then to build a model of each distribution. While it is possible to search the best matching distribution or to fit the CDF, we presently prefer to keep the exact CDFs corresponding to discrete data, without transforming it to continuous fitted functions (Fig. 8).

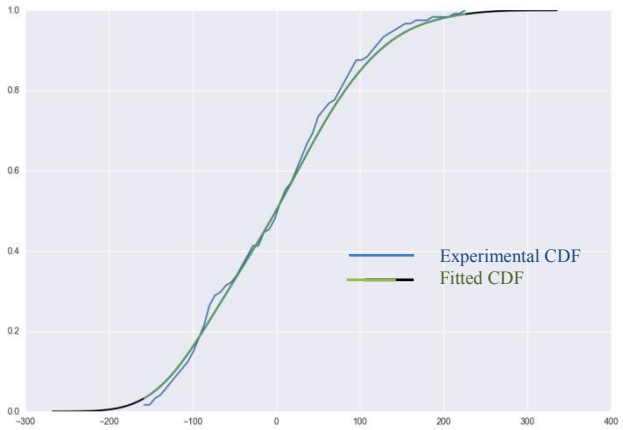


Figure 8: First coefficient CDF

2.4 Generation

Even though the coefficients are uncorrelated (not shown), these coefficients can be dependent in a more complex way. Therefore, the generation process has to take into account the dependence. Since the coefficients are of different marginal distributions, this cannot be done by only using a multivariate distribution, which suffers from the restriction that the marginal should be of the same type. One efficient way to do this is copula functions [28].

That is, copula functions allow one to model the dependence structure independently of the marginal distributions. Any multivariate distribution function can serve as a copula. That offers a good modelling flexibility.

For our generation process, we use the Gaussian copula, since two parameters (Mean and correlation matrices) are enough to describe it. The algorithm is explained in details in [21, 22, 25].

2.5 Validation

To validate our approach, we generate different sets of 300, 500, 800, 1000, 2000 and 10000 virtual grains. Surfaces, volumes and mean radius distributions are then computed and compared to those of the original data. (Fig. 9) shows the results, and Kolmogorov-Smirnov tests results are presented in Table 2.

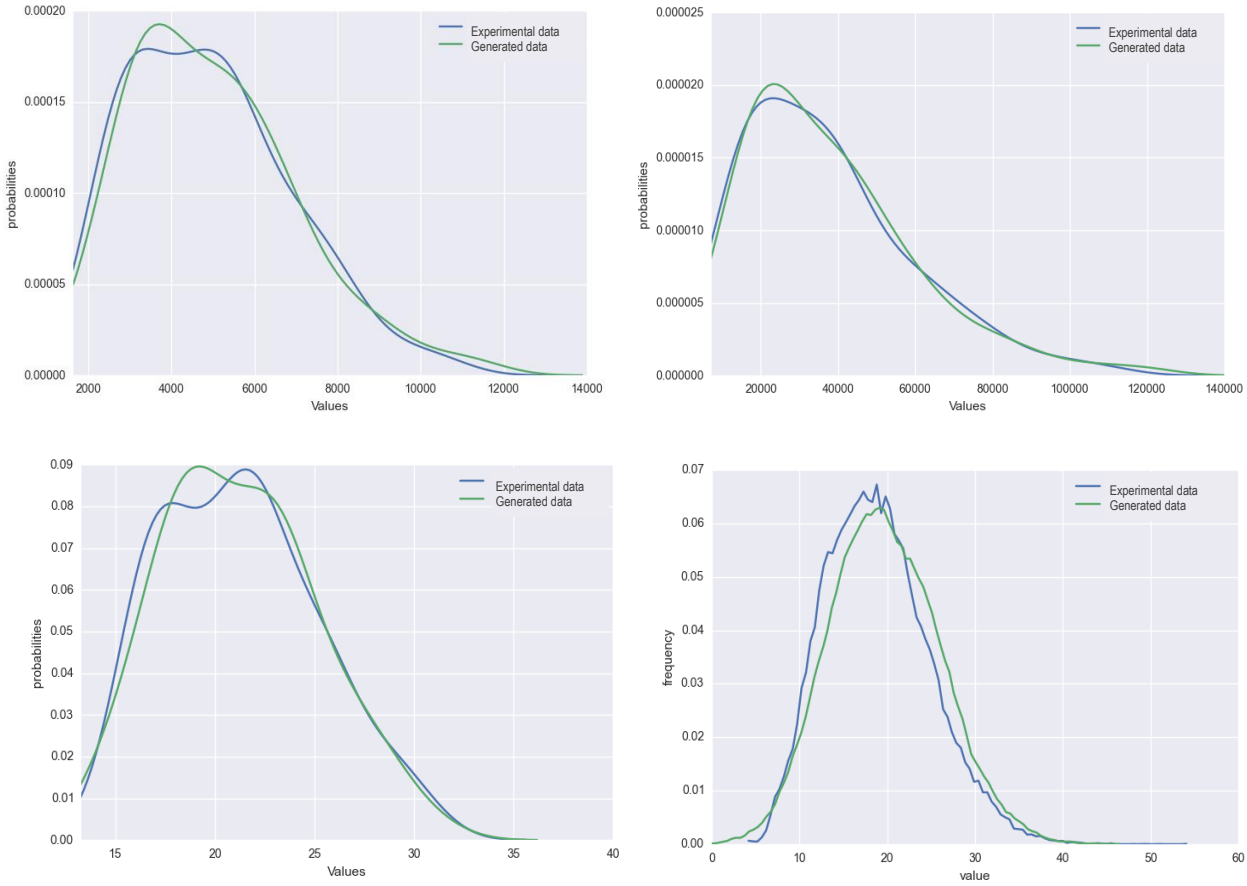


Figure 9: Sample validation – 10000 grains generated

Table 2: Values of Kolmogorov-Smirnov tests between original generated data S, V, Rm distributions

Number of generated grains	KS Surfaces	KS Volumes	KS Rayons moyens
300	0.949	0.949	0.811
500	0.993	0.993	0.831
800	0.994	0.994	0.883
1000	0.998	0.939	0.705
2000	0.976	0.896	0.870
10000	0.939	0.968	0.613

By analysing Fig. 9, we see that for surfaces, volumes and average radii, the peaks are the points that match the least. That can be explained by the fact that the real particle dataset (121 grains) is relatively small, and insufficient for estimating accurately statistics of the grains shape, and hence capturing all shape features. That was proved by Liu et al. [18] who analysed the impact of data set size on the accuracy of results using spherical harmonics approach, and by Grigoriu et al. [9] who also proved the insufficiency of a dataset of 128

aggregates to exactly represent the concrete grains shape. They showed that a “small data set was unable to accurately estimate statistics of aggregate geometry beyond second-moment properties and marginal distribution”.

However, the high values of KS tests obtained and the representations show that we get satisfactory results, even with a small data set. That confirms the accuracy of the approach and shows that enriching our data set will certainly allow to get an even better and exhaustive characterization of ballast shape, and offer an interesting transition between real and virtual grains in order to incorporate them in DEM simulations.

3 ILLUSTRATION

As shown previously, POD procedure allows to very well approximating the grains shape through eigenmodes and coefficients. One interesting question would be how to link eigenmodes and coefficients to shapes features.

One of the advantages of this method is ordering the dominating features by decreasing order (first modes have the biggest contributions to energy of the system, and the largest values of variance). We then expect the first mode to hold an important part of shape features (with 45% of the energy of the system).

To observe the evolution of grains shape through modes, we represent the same grain reconstructed with the first 1 (energy = 45%) to 20 modes (95%) in Fig. 11. We can see the progressive emergence of shape details as we add new modes. As the quantity of information increases (error decreasing), we minimize the sum of the squared differences of the distances between the point on the real grain and the same one represented with a finite number of basic functions.

The first fourth modes are shown in Fig.12. We see that the first mode, contributing most to the energy of the system, has a complete shape of a grain while the rest of the modes constitute the other details of shape.

Finally, we represent reconstructed grains with only the first mode in Fig. 13. For all 121 grains, we have a “round” shape.

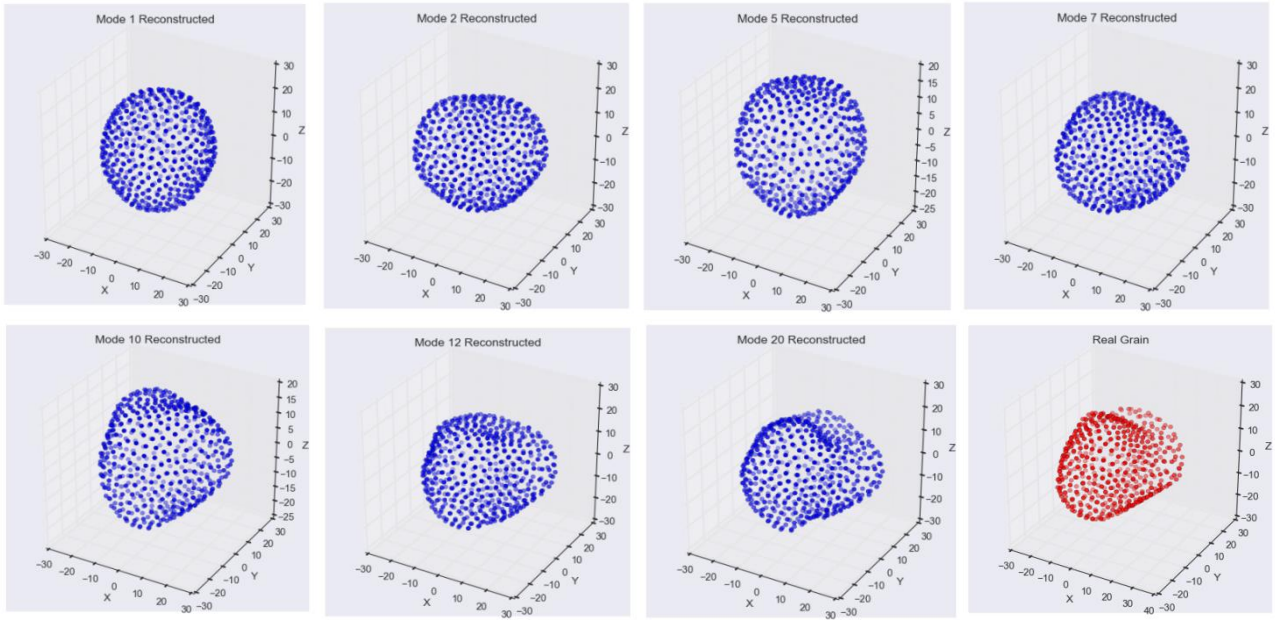
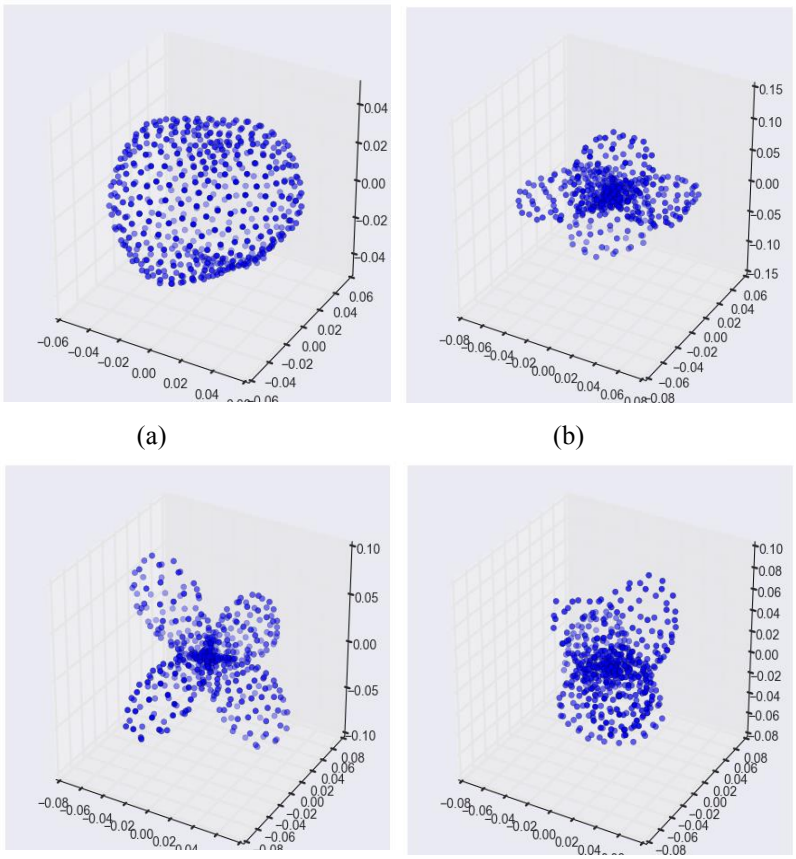


Figure 11: Grain shape evolution through modes 1 to 20 and real grain



(a) (b)

(c) (d)

Figure 12: (a) Mode 1 (b) Mode 2 (c) Mode 3 (d) Mode 4

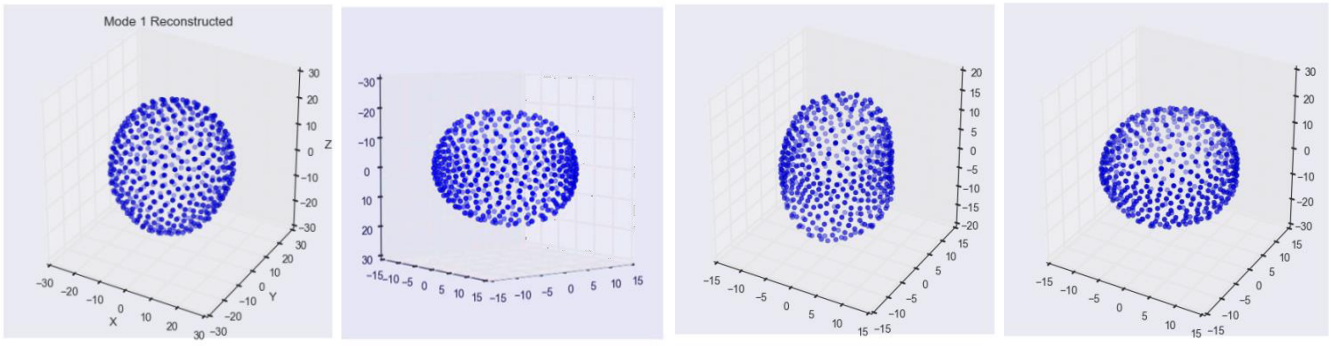


Figure 13: Different grains reconstructed from mode 1

3 CONCLUSION AND PROSPECTS

An innovative approach, based on dimensionality reduction by means of POD, leading to an optimal and nearly exhaustive shape characterization of real ballast grains has been presented. A method to generate sets that are representative of real grains has also been introduced, and validated by comparing some properties of the grains, such as surfaces and volumes. The method proved to give satisfactory results, and will give even better results for a data set of a larger size, as it will more accurately capture shape features. By observing the grain shape evolution through POD eigenmodes, studying more the link between the latters and shape features can be an interesting future outlook.

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