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A SIMPLISTIC GEOMETRIC APPROACH TO GENERATE RANDOM SPHERE PACKS FOR SELECTIVE LASER MELTING SIMULATIONS

Luca Luberto[1,a] **and Kristin M. de Payrebrune**[1,b]

[1] Institute for Computational Physics in Engineering
Technische Universität Kaiserslautern
Erwin-Schrödinger-Str. 56, 67663 Kaiserslautern, Germany

[a] E-mail: luca.luberto@mv.uni-kl.de

[b] E-mail: kristin.payrebrune@mv.uni-kl.de

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Abstract. In selective laser melting, components are produced by layer-by-layer melting of a powder bed. To investigate the interaction between the powder bed and the laser energy in the process, it is necessary to generate different powder bed configurations with a defined particle size distribution. For this purpose, based on different particle contact approaches, a simple algorithm for planar particle bed configurations was developed in the Julia programming language. Based on the so called 0- and 1-particle-contact approaches, a monodisperse sphere packing with a filling ratio of up to 64%, and with a normally distributed particle size with a filling ratio of up to 67% were generated. With the 0-particle-contact approach, the individual powder beds could be generated more quickly, but showed an insufficient degree of filling. In contrast, the 1-particle-contact approach can produce powder beds realistically. An extension for spatial problems, as well as variations in the contact approaches, is given by the simple algorithm design and shall be implemented and further investigated in simulations of selective laser melting.

1 INTRODUCTION

Selective laser melting (SLM) is an additive manufacturing process. In this process, a powder material is locally melted by a laser and, after a short cooling time, forms a coherent solid structure [1]. Due to the manufacturing tolerances of the particles, their size in the powder bed is subject to statistical variation, shown in figure 1 by [2]. This leads to irregular powder beds, which, in the worst case, increases defects, such as pores or cracks [3] and thus strongly affects the performance of the finished part. In order to simulate the SLM process realistically, the powder bed and its properties, such as its particle size distribution, must be generated. One challenge in modeling is that the particle-to-system size difference is often several orders of magnitude, such that suitable simulation methods are needed or appropriate assumptions must be made.

Two basic approaches can be distinguished for the generation of powder beds [4]. In the so

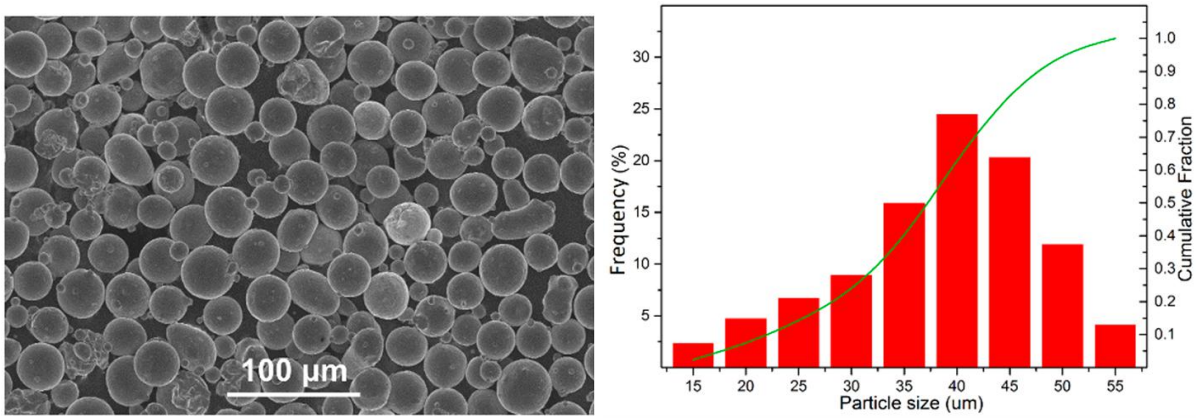


Figure 1: Left, scanning electron microscope (SEM) image and corresponding particle size distribution right of Ti6Al4V particles [2]

called dynamic approach, the generation of the powder bed is done via a discrete element method (DEM) simulation, where Newton's equations of motion and a contact model for each particle are solved [5]. DEM simulations are also suitable for complex geometries as well as various material pairings, but they are very computationally intensive. In the second, called geometric approach, all methods are based only on geometric calculation and constructions. Thus, in contrast to DEM, the powder bed can be generated faster and more efficiently. However, with the geometric approach, no interaction of the individual particles or different material interactions can be taken into account. Various studies can be found for both approaches. Thereby, the dynamic approach is often used as an initial preprocessing step for SLM process simulations [6–8]. In contrast, the studies concerning the geometric approach strongly address the particle bed characteristics and often have no explicit reference to a process simulation [4, 9–11].

This paper deals with the generation of a two-dimensional powder bed by a geometric approach based on the Julia programming language [12]. For the particle generation, a size distribution of the powder is first defined. Then, the particles are randomly placed in the packing region using different particle contact approaches.

The work is divided into four major sections. The properties of a powder bed are covered in the first section. The explanation of the algorithm is provided in the following section. The algorithm's appropriateness is tested in section three. The work is wrapped up in the conclusion, which is the last section.

2 POWDER BED CHARACTERISTICS

A powder bed can be characterized according to different criteria. In the present work, this is done according to three criteria: particle size distribution, packing density and coordination number. The particle size distribution serves as input for the algorithm. The packing density and coordination number are indicators for the quality of the powder bed and are only determined in a post-processing step. In the following, the criteria are explained in more detail.

The particle size distribution (PSD) represents the statistical fluctuation of the particle size in the powder bed [2]. The modeling of this quantity can be done with probability density

functions. In this work, a normal distribution

$$r \sim \mathcal{N} = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\frac{(r-\mu)^2}{\sigma^2}\right)$$

with the mean particle size μ and its standard deviation σ to model the variation in radius r. The packing density ϕ is defined as the ratio of circular area to total area. For the plane case and for N particles, the packing density is calculated via

$$\phi = \frac{1}{A_T}\sum_{i=1}^{N} A_i.$$

Here A_i is a single circular area and A_T is the total area.

The coordinate number cn represents the average number of contacts in the powder bed between two particles and is defined by

$$cn = \frac{1}{N}\sum_{i=1}^{N} C_i.$$

C_i is the contact parameter, which is $C_i = 1$ if contact between two particles exist and $C_i = 0$, in all other cases.

The powder bed in selective laser melting is not compacted during the application process. For this reason, the algorithms and studies presented in this paper refer to the generation of a so called loose particle bed.

3 ALGORITHM

The algorithm used to generate a planar powder bed is based on the geometric approach. A mesh grid in combination with a so called ball tree is used as data structure [13]. To generate this special data structure, the individual grid points of the grid are subdivided into intersecting and nested hyperspheres. This subdivision leads to fast accessible specific grid points, which is of great advantage especially for later collision checking.

To approximate the defined particle size distribution best, the circular particles are generated with the previously selected probability density function of the radius. In each step the algorithm then tries to place the new particle based on the selected particle contact approach and collision check in the domain. If no suitable location for the particle is found within n_T iterations, a particle with new radius is generated. Thus, the particle contact approach and the collision check form the core of the algorithm, which will be explained in the following section.

3.1 Particle contact approach

The contact conditions can generally be differentiated in 0-particle-contact, 1-particle-contact and 2-particle contact approaches. The approach of 0-particle-contact is a kind of brute force method, since it searches only for free locations in the domain. The position for a new particle

is generated via a random vector and checks only if the new particle does not touch another one. This method can generate particles very fast, especially in the first generation phase, when the packing density is low, but slows down strongly with increaseed packing density. Furthermore, this approach does not guarantee contact with other particle, which can lead to many pores in the powder bed. In contrast, the 1-particle-contact approach guarantees contact with at least one existing particle. During each generation step, an existing particle is randomly selected and a construction circle calculated with radius of selected and new particle. In a next step, a predefined number of angles between 0 and 2π are generated and stored in a vector in a random order. Based on this vector, a position is searched for which the new particle does not intersect any other particle but touches it in one point at most. Since in the worst case, all angles are tested for a new particle location, this procedure is more complex in comparison to the 0-particle-contact approach. However, unused empty spaces are better avoided and powder chains with higher density can be generated. With the 2-particle contact approach two contact points are guaranteed. This method is based on the solution of a nonlinear system of equations to determine the center coordinate of a new circle. The choice of two particles attached to each other is again random. The system of equations to determine the coordinates (x_3, y_3) for the new particle (cf. Figure 2 right are

$$(x_3 - x_1)^2 + (y_3 - y_1)^2 = (r_1 + r_3)^2$$
$$(x_3 - x_2)^2 + (y_3 - y_2)^2 = (r_2 + r_3)^2.$$

This approach guarantees a very tight packing due to at least two contacts guaranteed, but solving the system of equations is very time-consuming. Due to the time-consuming operations, this approach is not considered further in the study.

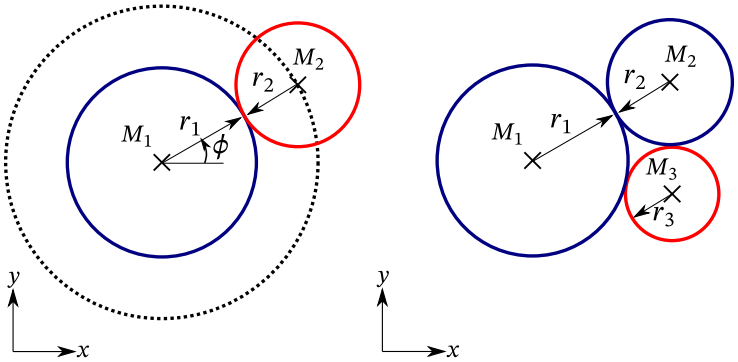


Figure 2: 1-particle-contact approach left and the 2-particle contact approach right. Newly generated particles are displayed in red.

3.2 Collision check

A collision check is part of each particle contact approach. This is done by discretizing the area by grid points, which are initially assigned to the values $s_g = 0$. As soon as a circle is finally

placed, the value $s_g = 1$ is assigned to each grid point lying in the circle. For every new circle, the collision detection checks whether grid points in its interior already belong to another circle by summing up the status values of the grid points

$$\text{col} = \sum_i (s_g)_i \quad i \in \bigcirc.$$

As soon as the collision sum col > 0 the new circle intersects an old one and the position is invalid. Figure 3 on the left shows the case of an infeasible position with collisions labeled by an cyan colored circle. Specifically, this example results in a collision sum col = 8. A new position is determined based on the chosen particle-contact approach. In the right figure, all grid points have the status $s_g = 0$, so col = 0 and the found position is valid.

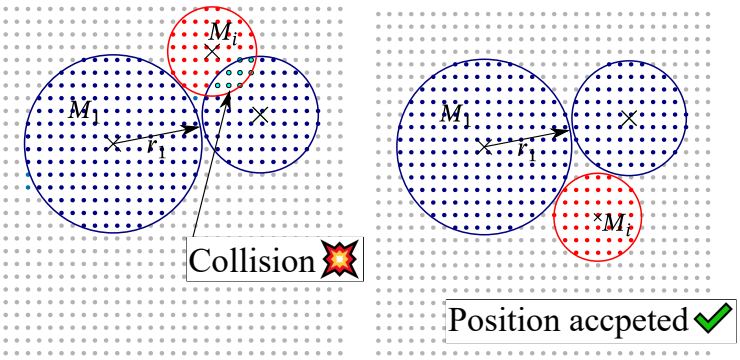


Figure 3: Example on the left shows an infeasible scenario, with the collision sum col = 8. Example on the right shows a feasible scenario, the collision sum here is col = 0.

The entire code to generate a planar powder bed was realized with the Julia programming language, version v1.6.3. In addition to the fast execution speed, the language is characterized by a MATLAB-like syntax, which guarantees integration in the in-house model of the selective laser melting process. The data structure and the query for collision are based on the package `NearestNeighbors.jl` by Carlsson [14].

4 STUDY

In order to test the different methods we studied 100 samples of planar powder beds generated with the 0-particle-contact and 1-particle-contact approach and their resulting particle number, packing density and coordination number. First, powder beds with constant radius are generated (monodisperse powder bed). Second, more realistic powder beds for selective laser melting with a defined particle size distributions is generated. For all studies, a square surface with side length of 4.0 µm at a resolution of 0.015 µm was used. The powder parameters are listed in the respective sections.

4.1 Monodisperse Powder Bed

For the generation of the monodisperse powder bed, the powder parameters from Table 1 are used. The goal is to generate monodisperse powder beds with a packing density of 0.634 -

0.65 [15]. Figure 4 shows an exemplary configuration and the corresponding contacts between particles in the powder bed for both approaches. Figure 5 shows histograms for the 100 samples in terms of particle number, packing density and coordination number.

Table 1: Powder parameters for the monodisperse powder bed

Distribution	-
Mean radius	0.075 µm
Standard deviation	-

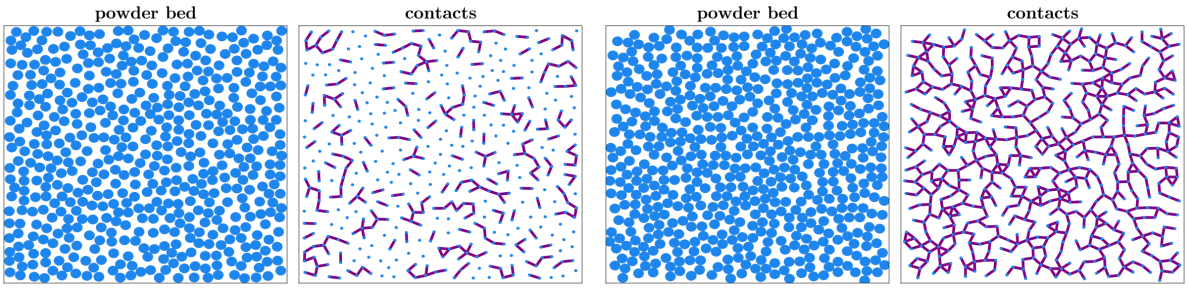
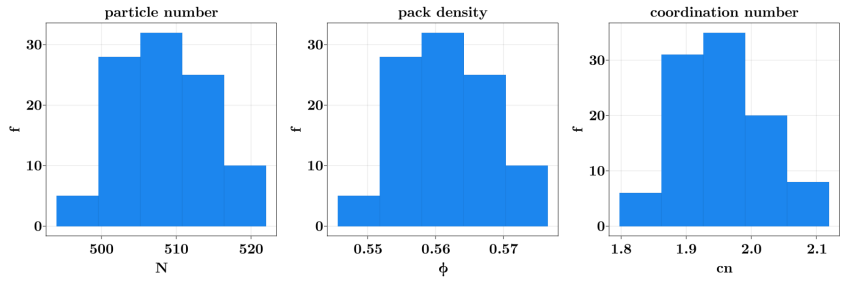


Figure 4: Example configuration with associated contacts for a monodisperse powder bed from the study.

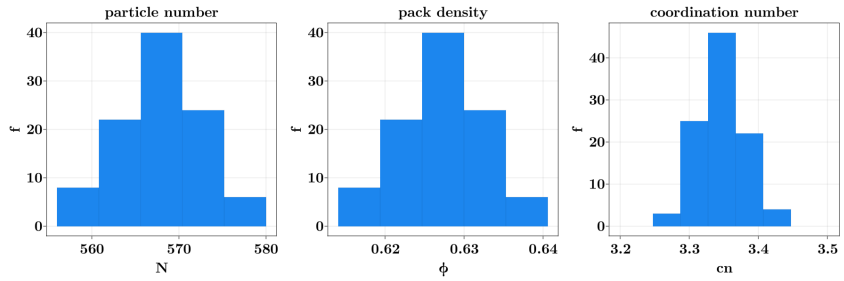
The differences between the two approaches can be seen in the exemplary configurations. With the 0-particle-contact approach, significantly fewer contacts are generated than with the 1-particle-contact approach. Accordingly, less particles and a lower packing density are to be expected. This is clearly visible in the histograms, where the differences can be seen across all samples. The packing density for the 0-particle-contact approach is in the range of 0.55 - 0.57, with 500 - 520 generated particles and a coordination number of 1.8-2.1. In contrast, with the 1-particle-contact approach a packing density of 0.62 - 0.64 can be achieved, which is in agreement with the literature. Thereby, the coordination number is 3.25-3.45, with significantly more generated particles between 560 and 580. Even though the 0-particle-contact provides a significantly lower packing density, it still can be used as first attempt of a powder bed for SLM simulation. However, if a higher packing density than 0.6 is required, a generation by the 1-particle-contact approach has to be done.

4.2 SLM Powder Bed

In this study, the main focus is on a proper approximation of the particle size distribution, in the powder bed. For this purpose, a Gaussian distribution is now assumed for the diameter of the particles. To avoid extremely small or large particles, a truncated Gaussian distribution limits the sampling of the diameter between 0.015 µm, and 0.15 µm. All powder parameters used are summarized in Table 2. Figure 6 shows again an exemplary configuration and corresponding



0-particle-contact approach



1-particle-contact approach

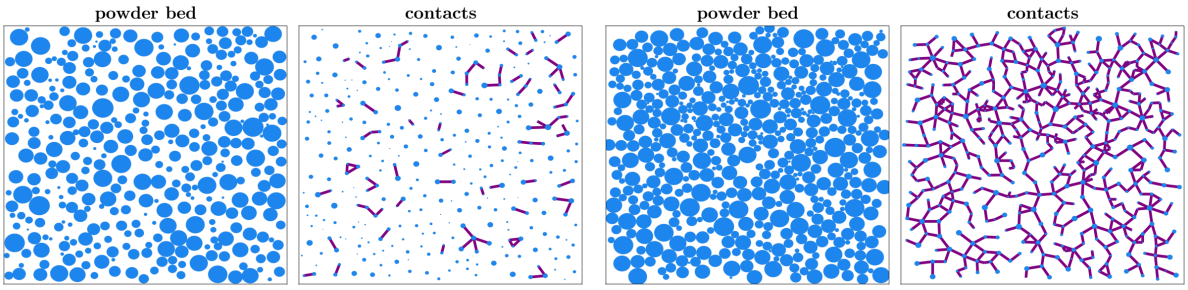
Figure 5: Histograms of particle number, packing density and coordination number for 100 samples. Top for the 0-particle-approach, bottom for the 1-particle approach.

contacts in the powder bed. Figure 7 shows the related histograms for the 100 samples in terms of particle number, packing density and coordination number.

Table 2: Powder parameters for SLM powder bed generation

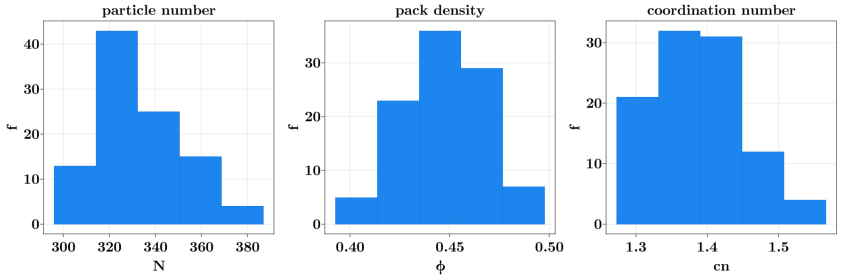
Distribution	Truncated Gauss (0.015 µm, 0.15 µm)
Mean radius	0.075 µm
Standard deviation	0.0375 µm

For the generated SLM powder bed shown in figure 6, the differences between the two approaches are more obvious. With the 0-particle contact approach, there are extremely many gaps and hardly any contacts to the neighboring particles, whereas the powder bed with the 1-particle contact approach generates many contacts with the desired or even higher density. However, neither approach completely fills the boundary areas. Considering the histograms in figure 7, the differences between the two approaches become even more obvious. The 0-particle contact approach can only place 325-425 particles in the domain, resulting in a low particle density of 0.42-0.52. Accordingly, the coordination number ranges from 1.3-1.5. In contrast, the 1-particle contact approach places 525-575 particles in the domain. The higher particle number leads to more contacts between particles, which is reflected in a coordination number between $3.3 < cn < 3.45$ and a much higher particle density with 0.68-0.72, which is even higher than the desired density from the literature.

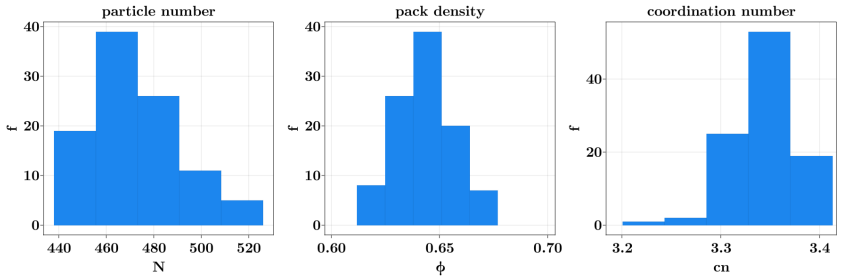


0-particle-contact approach 1-particle-contact approach

Figure 6: Example configuration with associated contacts for an SLM powder bed from the study.



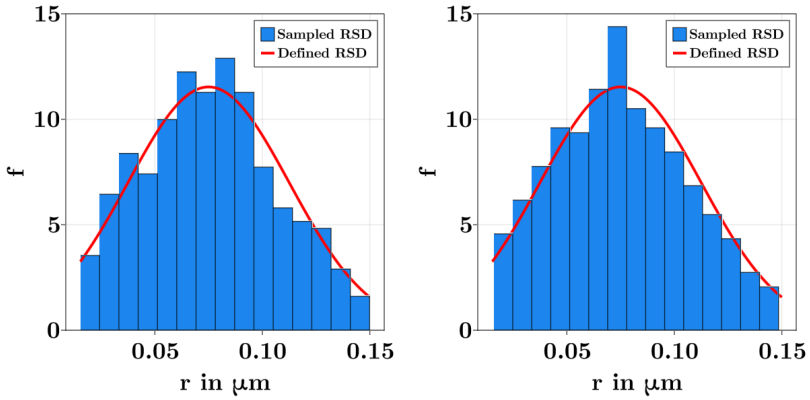
0-particle-contact approach



1-particle-contact approach

Figure 7: Histograms of particle number, packing density and coordination number for 100 samples. Top for the 0-particle approach, bottom for the 1-particle approach.

Figure 8 shows the predefined size distribution in red and the abundance of the different powder sizes for the examplarly configuration. Here, a good approximation of the defined size distribution can be observed for both approaches, which is explainable by the amount of placed circles. However, due to the many voids the 0-particle approach should not be used to generate powder beds for SLM simulations.



0-particle-contact approach 1-particle-contact approach

Figure 8: Size distribution of the example configuration with associated contacts for an SLM powder bed from the study.

5 CONCLUSIONS

In this study, an algorithm for generating planar powder beds for selective laser melting is presented, with focus on a good approximation of a realistic particle size distribution. By using simple particle contact condition, the algorithm is very well understandable. The operation and differences of the 0- and 1-particle-contact approach are tested in this study. First, a monodisperse powder bed was generated with both approaches resulting in relatively dense packings. However, the density from literature of 0.634 - 0.65 could only be achieved by the 1-particle-contact approach. The characteristic values for the particle and coordination numbers for the 0-particle-contact approach were correspondingly and significantly smaller as for the 1-particle-contact approach. In the second study, an attempt was made to generate an exemplary SLM powder bed with a defined particle size distribution. Here, the differences between both approaches are more obvious: the packing density as well as the number of particles and the coordination number of the 0-particle contact approach are not sufficient to represent a loose particle bed for an SLM process. In contrast, a realistic powder bed with high packing density and many particles can be generated with the 1-particle-contact approach. The approximation of the predefined particle size distribution are possible with both approaches. In summary, the 0-particle-contact approach can still be used for monodisperse powder beds, but is not sufficient to generate a realistic powder bed of an SLM process. However, a combination of both approaches is promising, since the positive characteristics of the respective approaches can be used independently in different generation phases. Likewise, a further condition for sampling near the edge can increase the packing density.

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