Modeling of Powder Bed Processing – A Review

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Abstract

Many models have been developed to model powder beds and these methods can be implemented to model a powder bed for Selective Laser Sintering, Selective Laser Melting and any other technique of additive manufacturing which uses powder beds. Two of the main systems are the Discrete Element Method (DEM) and the Geometric Method. The purpose of this paper is to analyze each of the methods. It will first highlight how each of the models creates the powder bed. The next aspect reviewed is the computational time and its causes. And lastly, each of the methods will be examined for their accuracy as shown from various experiments that have been reported in literature. In addition to these methods, there are several others that have been proposed that will also be studied and compared to highlight the strengths and weaknesses of each.

Introduction

Multiple fields of science are interested in the simulation of a powder bed for various different applications; some of these fields include physics, chemistry, and engineering. Each of these areas of science have their own needs for what data is to be collected from the models that they create. Since there is such a wide range of needs for the data being collected, there is as also a wide range of need for the types of models that are in the literature. Most of the models studied assumed that the powder particles could be represented by perfect spheres. This would help to simplify the calculations performed by the system. Another generalization that can be made about the various systems is that the powder particles are incompressible. This results in again a much simpler and easier to implement model. When reviewing these systems, there are several aspects which can be compared to determine which method is best for each application. The main controls that are analyzed are the computational time required and the mechanical properties of the powder bed created. In addition to these main model characteristics, the results from the various models are compared to experimental data to validate their results. This validation is two-fold. The first piece of data used to validate the simulation is the packing density of the model. This is done by taking the total volume of the spheres and dividing it by the volume of the powder bed, which is the complement of the void fraction. The other benchmark which is used to determine the effectiveness of a model is to calculate the average coordination number. The coordination number is the number of contacts that a particle has with its surrounding particles. Therefore, the coordination number of a powder bed is the average coordination number of all of the particles. This value is very difficult to determine experimentally, therefore it is commonly used to compare various models and not used to

validate them. Overall, these two parameters are used to determine the effectiveness of a model and to compare models.

The models reviewed here only take into account the creation of the powder bed. There are several models in research which will model not only the creation of the powder bed, but will also model the melting of the powder particles and the creation of the final product. One representative paper is by King *et. al.* [1] which starts by laying particles over a Cartesian mesh background. Once the powder bed is created, several mechanisms are utilized to model the melting and other processes which occur. Some of the main processes included are: absorption, vaporization, capillary forces, gravity, convection, conduction, phase transformation, and many others. This model will first create the powder bed and then calculate the effect that the laser imposes on the powder particles based on these forces. This paper [1] is similar to other papers such as [2], [3] and [4] which all have some variation of modeling process which predicts the finished product. These models are not reviewed in depth in this work due to a slightly different focus. This research is focused solely on the creation of the powder bed. Therefore, the information in this paper is the foundation on which the other research can be conducted.

Discrete Element Method

The use of the discrete element method (DEM) began in 1979 by Cundal *et. al.* [5]. Their new method was to track the contact forces of a given particle throughout the entire simulation process. This idea has integrated itself into the simulation of powder beds. There are several different approaches that have been used in an attempt to model a powder bed using this method. Each of the DEM models starts out in a very similar way. To begin either one particle is selected and placed arbitrarily above the container as in [6] or multiple particles are generated and placed over the container as in [7]. These particles are selected to have different distributions. Some of the more rudimentary approaches use a mono-sphere approach. The more elaborate models use a distribution of radii to determine the size of the particles. The most common distribution is a normal distribution centered on the mean particle size. Once the particles are created, they are released and allowed to fall depending on the forces that are being used by the current simulation. All of the models that were found had several of the basic forces in common but, in an attempt to increase the accuracy of the model, some authors have added other forces which manifest themselves in smaller amounts. To begin, the major forces which are present in all of the simulations include the force of gravity, contact forces, and the force of friction. In most cases these are represented by Newton's second law of motion which is shown in equation 1. [8]

$$m_i \frac{dv_i}{dt} = F_i \quad I_i \frac{d\omega_i}{dt} = T_i \quad (1)$$

Where translational and angular velocities are represented by v_i and ω_i respectively. I_i, F_i, m_i and T_i represent the moment of inertia, total force, mass and torque of particle i. Using Newton's

laws of motion the forces of friction, gravity, and contact forces can be determined. These forces are then summed to determine the total forces on the particles.

Some of the authors have then added some interaction forces to increase the accuracy of their model. The two methods of calculating the interaction forces that have been found in the literature are the use of Van der Waals forces and JKR interaction model. The Van der Waals forces which are used in [6] are shown in equation 2.

$$F_i^v = \frac{AR}{12h^2} n_i \quad (2)$$

Where A is Hamakers constant, which is material dependent, n is the number of particles, h is the distance between the particles, assuming that they are of the same size with radius R. The other method of computing the interaction forces is to use the JKR. This model of interaction was developed in [9] and used by [7] in the modeling of powders. Equation 3 outlines the three main equations governing these interactions.

$$F_{ikr} = \frac{4E^*}{3R^*} a^3 - 4\sqrt{\pi\gamma a^3 E^*} \qquad \frac{1}{E^*} = \frac{1-v_i^2}{E_i} + \frac{1-v_j^2}{E_j} \qquad \frac{1}{R^*} = \frac{1}{R_i} + \frac{1}{R_j} \quad (3)$$

Where v is the Poisson ration, E is Young's modulus and E^* is a modified Young's modulus, R is the radius of every sphere in contact and R^* is a modified radius, α is the contact radius, and γ is the surface energy. Many of the researchers prefer to use the Van der Waals forces due to the ease with which it can be implemented into the model. However, this model cannot take into account any deformation that might occur due to strong interactions. That is why some researchers have used the JKR model to simulate the interaction forces.

Once all of the forces have been summed, it is simple to determine the direction and velocity at which a given particle will be moving. These particles would then be moved depending on the time step that was applied. Some of the authors, such as [6], used a constant time step which was found by using trial and error. This method works but either wastes computational time when particles are not interacting very much or, does not have a high resolution when the particles are interacting a lot. Therefore, one of the authors [10] used an adaptive time step which will only allow a particle to move a set amount and will not allow a change in force greater than a given amount. This will result in less time lost computing when the particles are not interacting much. Overall, DEM is a robust model which can be applied to multiple situations but is very computationally expensive. A representative group of papers is listed in Table 1 to demonstrate the results which were found. It should be noted that [6] is only simulating the powder bed in 2 dimensions, as opposed to 3 dimensions like the other papers. It has been stated in [6] that this could increase the packing density by approximately by 25%. Other DEM simulations that were found included [8], [11], and [12], all of which had the components similar to these DEM simulations and only varied slightly in their approach and the conclusions which they were attempting to draw.

Table 1: Summary of common DEM simulation

Author	Forces Used	Results
Siiriä, *et. al.* [10]	Gravity, Contact Forces between particles and between particles and walls, friction between particles and between particles and wall	Highest packing density 0.55. Friction coefficient had largest effect on the particle packing density
Cheng, *et. al.* [6]	Gravity, Contact Forces between particles and between particles and walls, friction between particles and between particles and wall, Van der Waals interaction forces	Highest packing density 0.8696 which did not take into account Van der Waals forces or friction. Van der Waals interaction forces and friction reduced the packing density substantially.
Deng, *et. al.* [7]	Gravity, Contact Forces between particles and between particles and walls, friction between particles and between particles and wall, JKR interaction model	As the particle diameter is increased the density begins to reach equilibrium at 0.4 but, with smaller particles the density could be as high as 0.85

Geometric Models

Another prevalent model which is used to simulate the creation of a powder bed is known as the geometric model. There are several different algorithms in the literature which are meant to create a powder bed quicker than the DEM models. For this review, two methods will be outlined, but more can be found in [13], [14], [15], and many others.

The first model outlined is by Han *et. al.* [16], which is referred to as a compression algorithm. To begin this method, the direction of compression must be given. Once this direction is given, the volume to be filled with particles is filled with spheres randomly so that there is no overlap between any of the particles. This is shown in figure 1a as the red spheres. When this is completed, the volume is filled but the density is extremely low. The next step is to compress the spheres together. To do this a list of the neighboring spheres of each sphere is created and the distance which a sphere can move in the compressive direction is calculated. The space is then updated, which moves the particles the smallest distance of all of the particles. This is repeated until the difference in the initial and final potential energy is below a given tolerance. Once the particles have been compressed, a shaking algorithm is implemented. This algorithm is similar to the compression except the compression direction is randomly selected from a set range of angles centered on the direction of compression. This will ensure that the particles are at their absolute minimum potential energy. This can be seen in figure 1b where all of the spheres are now at the bottom of the container. This process is then repeated starting with refilling the container until the container is full. A schematic can be seen in figure 1 which demonstrated this process at work. In figure 1c the red spheres are those that have already been

placed and the green represent the refilling of the container. They are compressed in figure 1d. This is repeated until the container is finally filled in figure 1h. This model resulted in an extremely fast, 181 seconds, packing of over 26,000 spheres into a structure with a 0.5289 packing density.

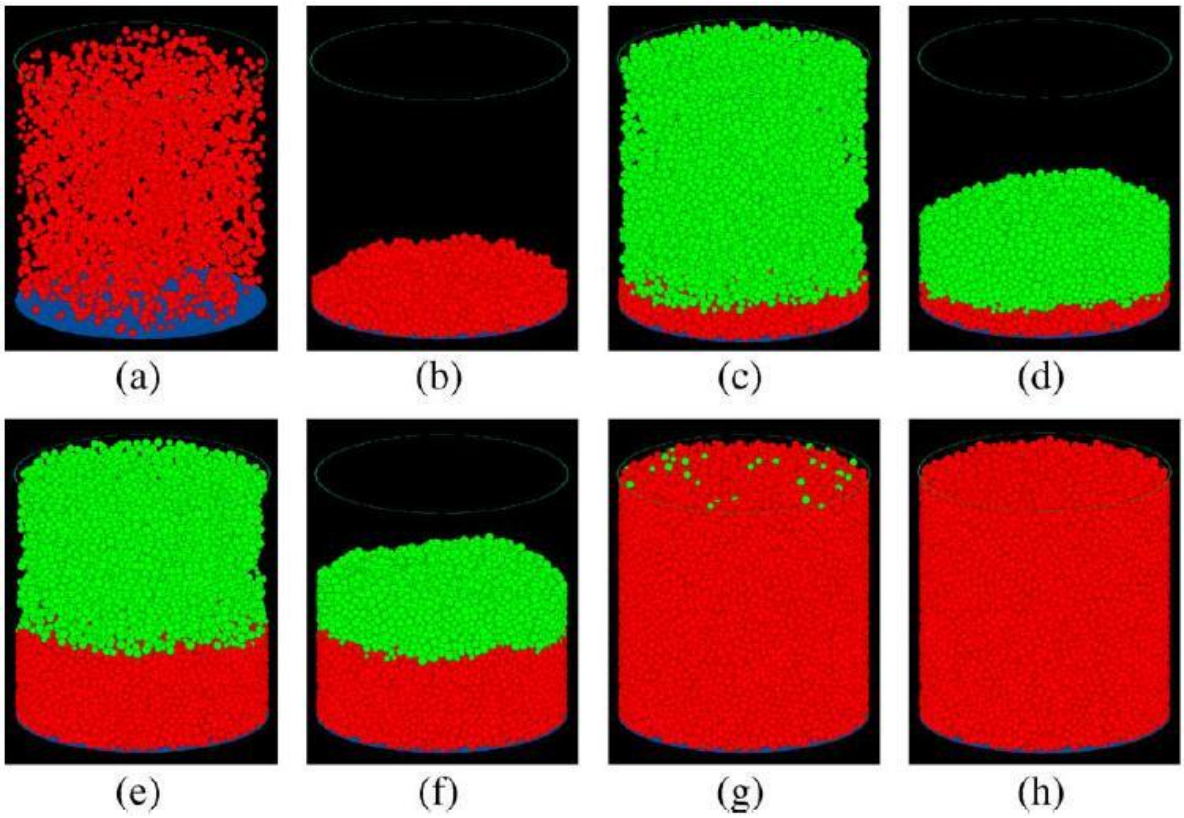

Figure 1: Schematic of compressive algorithm [16]

The other geometric method presented is from Jerier *et. al.* [17] and their method focused on a tetrahedral mesh into which the spheres are inserted. After this mesh is created spheres are added at the nodes and at the centers of the edges, this can be seen in figure 2a. The spheres which are on the nodes are given a radius which corresponds to the length of the shortest adjacent edge. Whereas, the spheres at the center of an edge are given a radius of L/8 where L is the length of the edge on which they are positioned. If these given radii are outside of the predefined r_{max} and r_{min} then the radius is either set to a random number within the range if it is too large or, set to r_{min} if the radius is too small. Once this has been done, a sphere is placed at the barycenter of every triangle and tetrahedron in the mesh. The last step to obtain a loose packing is to place a sphere at the midpoint of the barycenter and the nodes of each tetrahedron, which will result in figure 2b. This results in a packing of the mesh which does not consider the boundaries of the mesh. To fix this problem virtual spheres are created which approximate the external planes of the mesh. Then, any sphere that contacts these spheres is eliminated, as seen in figure 2c. To obtain a greater packing density the structure is searched looking for the voids

which could be filled with smaller spheres. This is done by finding where four adjacent spheres create a tetrahedral. A fifth sphere is placed into the void which is created by the set of spheres, resulting in a much more dense packing which can be seen in figure 2d. If this step is left out then the packing density of this model is only 0.45. Overall, this method created a 0.75 packing density.

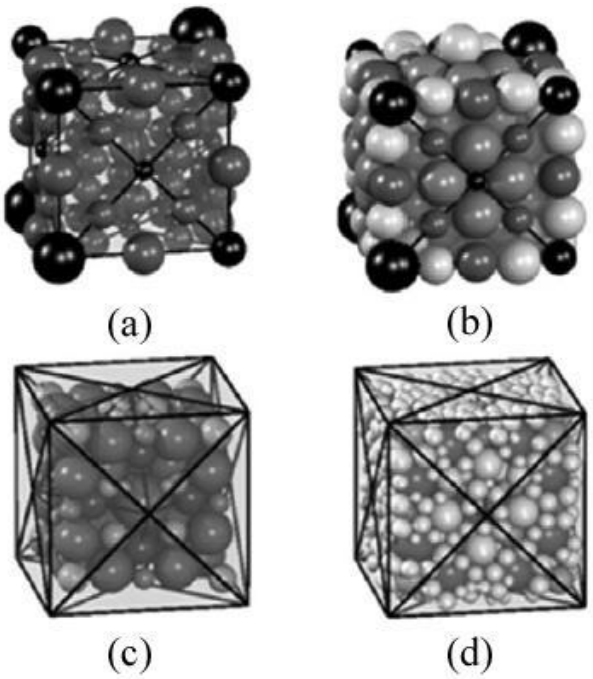

Figure 2: Steps for creating powder bed using tetrahedral mesh [17]

As can be seen from these two methods highlighted, in general the geometric method is a very computationally efficient method of creating a powder bed. A multi-thousand particle powder bed can be created in a matter of minutes as opposed to other methods which could take days. However this method does have its negatives. For starters, it does not create a mechanically stable powder bed. Another issue with this system is that it does not return the contact forces and other forces that are present within the system. For some applications this is the ideal way to model the powder bed.

Comparison of DEM and Geometric Models

When comparing these methods of modeling the powder beds there is no apparent way to determine which is the overall best method. Each of the systems has applications in different sectors of research. The basic similarities and differences are outlined in Table 2.

Table 2: Comparison of DEM and Geometric Simulations Features

	DEM	Geometric
Time per Simulation	Long	Short
Computational Efficiency	Low	High
Mechanically Stable	Yes	No
Inter-Particle Forces Recorded	Yes	No
Stresses Recorded	Yes	No

As Table 2 outlines, there are several different parameters that can be used to compare the various methods of creating a powder bed. The first is the amount of time and the computational power which is required. The geometric method exceeds the DEM method when analyzing these parameters. This is because there is much more computational power required to compute the forces within the powder bed. The means to evaluate these methods is to compare the computational times which are reported in several papers; this comparison can be seen in Table 3. Evaluating the table, one can see a drastic difference in the amount of time which is required for each of these methods. To create a powder bed using a DEM simulation it is expected that at least an hour will be used if a powder bed of more than a hundred particles is studied. Some methods are faster than others, but DEM is still a time-consuming method. On the contrary, when using a geometric method, the slowest method was able to create a powder bed, with an order of magnitude more particles, in less than 2 hours. This shows that if computational time is of the utmost importance then the geometric method should be the method of choice.

Table 3: Comparison of computational time of DEM and Geometric Methods

Author	Method Used	Results
Cheng *et. al.* [6]	DEM	2 hours for 9,000 spheres
Siiria *et. al.* [10]	DEM	1-10 hours for 100 spheres based on parameters used
Mueller [14]	Geometric	6,628 seconds for 61,991 spheres
Han *et. al.* [16]	Geometric	181 seconds for 26,787 spheres
Jerier *et. al.* [17]	Geometric	300 seconds for 35,000 spheres

Another mode of evaluating these methods is to compare the packing densities and coordination numbers reported in the various papers. To do this, a sample of the papers has been compared in Table 4 and Table 5 comparing the packing densities and coordination numbers respectively. When analyzing Table 4, it is clear that both of the methods yield packing densities that are similar to the experimental results. The main difference in these results is that the packing density of the DEM methods is only dependent on the forces which are used in the model. Since these forces are what dictate the packing density, the results are a better representation of the experimental results. This is in contrast to the geometric model which can create a powder bed with a specific packing density. In the geometric models, the packing density is used as a parameter which will stop the creation of the powder bed. This leads to the necessity of either

performing DEM simulations or experiments to determine what values are appropriate for the packing density to be used in the simulation.

Table 4: Comparison of packing densities of DEM and Geometric Methods

Author	Method Used	Results
Finney [18]	Experimental	Packing Density 0.636 (with particles of normal distribution)
Deng *et. al.* [7]	DEM	Packing Density 0.65 (with particles of singular diameter)
Siiria *et. al.* [10]	DEM	Highest Packing Density 0.55 (with particles of singular diameter)
Shi *et. al.* [19]	DEM	Stable Packing Density 0.578 (with particles of normal distribution)
Jerier *et. al.* [13]	Geometric	Packing Density 0.7-0.4 based on user inputs (with particles of normal distribution)
Mueller [14]	Geometric	Packing Density 0.59-0.37 depending on ratio of container height to particle diameter (with particles of singular diameter)
Han *et. al.* [16]	Geometric	Packing Density 0.5289 (with particles of normal distribution)

Table 5 compares the coordination numbers of the various methods. When reviewing a paper such as [20], it becomes obvious that there are multiple different values which have been reported in the literature. This has led to different results based on several parameters, the largest factor is the material used. For this reason, the value of the DEM solutions are usually assumed to be a more accurate estimate of the actual coordination number due to the method of the powder bed generation. As can be seen from the data which is displayed in Table 5, the DEM solutions produce a coordination number which is slightly smaller than that of the geometric models. The difference in these simulations can be again attributed to the methods used to generate the results. In the DEM simulation, the model is a more realistic representation of the actual method of building a powder bed. This results in a bed which has a coordination number more closely aligned with reality. In the geometric method, the coordination number can be varied within the model by changing the initial parameters which determine when the program will end. R.M. German in [20] reports that there can be a wide variance in the reported values based on the material and other variables. Therefore, this parameter should be used as a decisive factor with caution.

Table 5: Comparison of coordination number of DEM and Geometric Methods

Author	Method Used	Results
Deng *et. al.* [7]	DEM	Coordination Number of 4-6 varying on Particle diameter (10-1000um)
Shi *et. al.* [19]	DEM	Stable Packing Coordination Number 5.97
Jerier *et. al.* [13]	Geometric	Average Coordination Number 6
Jerier *et. al.* [17]	Geometric	Coordination Number 4.75-7.5 based on particle sizes

Due to the uniqueness of each model, various sectors of research rely on each of the models differently. One area of study that relies heavily on DEM simulations is the concrete industry. This area of research is very interested in the stresses that are felt by the particles of the concrete which dictated the use of the DEM simulations to find the state of each particle. On the other hand, for the use in modeling of powder beds for additive manufacturing it is usually only necessary to obtain a proper density and coordination number for the powder bed. Therefore, in most cases, the geometric method would be the best option because it is computationally cheap and has a short time per simulation; which would allow for more time and computation power to be spent on modeling of the thermal processes which are taking place within the system. The main problem with the geometric models is they contain an induced coordination number. In the modeling of the powder bed additive manufacturing systems this is crucial because the coordination number is one of the key factors which dictate the flow of heat through the powder bed. If a powder bed has a higher coordination number then heat will flow faster through the system, since heat travels faster by conduction than convection. This problem can be mitigated by selecting a geometric model which mimics the coordination numbers which are reported in the literature from DEM simulations.

Other Models

There are a few other models which are not as commonly used as DEM and the geometric method. These methods include, but are not limited to, the ballistic method powder bed generation, and the Monte Carlo simulation of powder beds.

The ballistic method for creating a powder bed can be found in [21], [22] and others. This model is a hybrid between the DEM and the geometric models. In this simulation a particle is selected and given a random radius, and x-y coordinates and placed high above the container. It is then moved down toward the powder bed until contact is made with either another particle or the floor. If contact is made with the floor the particle is considered at its final location. If it hits a particle then it is rotated about the place of contact until another contact is made. After this contact, the particle is rotated about these two points of contact until a third contact is made. This is then considered its final location. If the particle at any time contacts the floor or wall during these rotation it is then considered to be in its final location. This method allows for a much faster simulation than the DEM method and allows for a seemingly more random packing

of the particles. Based on the literature presented in [22] and the results presented, this method provides coordination numbers and porosities which are comparable to DEM simulation, geometric simulations, and experimental results.

Another approach to creating a powder bed that has been shown in the literature [23] and [24] is the use of Monte Carlo algorithms. Just as all of the other methods for powder bed creation this method varies depending on the author. In general, this method begins with filling a domain with a specific number of particles. These particles are given a random direction and distance to move. This motion is considered valid if the particle does not come into contact with a wall or another particle. This is considered a Monte Carlo step due to its use of random number generators to find the path and length. This Monte Carlo step is then repeated a given number of times. After the Monte Carlo steps are completed, the minimum distance between spheres is found to be δ. The domain is then scaled down by a factor derived from δ and the simulation is run again. This is method is completed until a specific packing density is created or the packing density between steps does not change more than a given threshold.

Conclusion

In general, all of these methods have been used to create powder beds which have been validated by experimental results. As was stated previously, the use of each method is dictated by the results which are desired from the simulation. The main factor which will determine the method used is the necessity of the contact forces. If these forces are required, then DEM is the only method which can be used. If these forces are not essential, then computationally it would be more efficient to use the geometric, ballistic, or Monte Carlo simulations. These last simulations would be the best for modeling of additive manufacturing powder bed systems due to their low computational time and accurate model. Overall, Table 2 can be used to help determine which method is the best for any given situation.

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