1 Discrete Element Modeling of Particle-Based Additive 2 Manufacturing Processes

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4 Abstract

A critical element for the design, characterization, and certification of materials and products produced by additive manufacturing processes is the ability to accurately and efficiently model the associated materials and processes. This is necessary for tailoring these processes to endow the associated products with proper geometrical and functional features. In an effort to address these needs in a computationally elegant and at the same time physically realistic manner, this paper presents the development of a methodology for simulating particle-based additive manufacturing processes which employs the Discrete Element Method (DEM). The details of the DEM-based methodology are presented first and the approach is demonstrated on a pair of test problems involving laser sintering of metal powders. The paper concludes with a discussion on how this approach may be generalized to broader classes of additive manufacturing systems, and details are given regarding future work which must be accomplished in order to further develop the present methodology.

5 *Keywords:* Additive Manufacturing; Layered Manufacturing; Rapid
6 Prototyping; Particle Methods; Discrete Element Methods; Laser Sintering;
7 Laser Accretion; Selective Laser Sintering; Selective Laser Melting; Direct
8 Metal Laser Sintering; Laser Cladding; Laser Engineered Net Shaping;
9 Electron Beam Melting; Direct Metal Deposition; Granular Dynamics; Powder
10 Metallurgy; Multiphysics; Heat Transfer;

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1. Introduction

Additive manufacturing (AM), also known as layered manufacturing or less formally as 3D printing, is an increasingly important technology for the production of a wide variety of components and structures. It consists of a broad family of fabrication techniques which are characterized by successive additions of material to a domain, as opposed to the repeated subtractions which are employed by most traditional fabrication technologies [1]. Recent years have seen a surge of interest in additive manufacturing technology from a broad number of engineering and manufacturing disciplines. This interest is primarily driven by the relative relaxation of geometric constraints provided by additive manufacturing methods; geometries which are difficult or impossible to produce by conventional means are often readily achievable. Additionally, the possibility of producing customized, low volume, or otherwise economically infeasible products [2] has stimulated much interest in the field.

Many of the most prevalent additive manufacturing technologies available at present are based on powders and the challenges associated with their modelling and simulation have been discussed elsewhere [3]. Typically, feedstock material in the form of a fine powder is introduced into the fabrication domain, followed by the directed application of energy to consolidate the powder into some solid form (e.g. sintering or melting). A conceptual example of such powder-based additive manufacturing is shown in Figure 1. While this methodology allows the production of geometrically complex components ranging from biomedical implants [4] to turbine blades [5], it introduces considerable complexity and uncertainty with respect to the material properties and associated functional response.

[Figure 1 about here.]

Because additive manufacturing processes operate in a spatially and temporally varying fashion, the material systems produced by these means can be significantly non-homogeneous, anisotropic, and nonlinear [6]. As a result,

1 additively manufactured products are beset by quality issues including dimen-
2 sional errors, delamination of layers, porosity and poor or indeterminate ma-
3 terial properties [7]. These issues are a substantial obstacle to the widespread
4 adoption of additive manufacturing, and often preclude the use of this technol-
5 ogy in performance-critical applications [7]. In order to address these issues, and
6 enable the development of design, characterization, and certification tools, it is
7 necessary to develop a methodology for the accurate simulation of powder-based
8 additive manufacturing processes and the resultant products.

9 In contrast to employing the numerical solution of the multiphysics partial
10 differential equations derived by first principles and the associated conservation
11 laws [3], in this paper we approach the challenge of simulating powder-based
12 additive manufacturing processes by use of the Discrete Element Method (DEM)
13 [8]. In particular, the principal goal of this research is to demonstrate the
14 feasibility of simulating powder-based additive manufacturing processes using
15 the DEM, even under a relatively simple set of physical approximations and
16 assumptions. The DEM is a numerical approximation method for mechanics
17 which is based on an interacting system of particles. These particles interact in
18 a Newtonian fashion, conduct heat transfer, respond to external fields, and may
19 form or break inter-particle bonds. By utilizing these physics encapsulated by
20 the DEM, we enable a simulation which captures the granular dynamics, energy
21 application, and consolidation aspects of powder-based additive manufacturing.

22 The history and background material regarding powder-based additive man-
23 ufacturing is the subject of Section 2, and a similar study of the Discrete Element
24 Method is found in Section 3. From this basis, we develop a general DEM for-
25 mulation for powder-based additive manufacturing problems in Section 4. The
26 details of this algorithm, such as collision detection, consolidation via bond for-
27 mation, and post-processing are discussed in depth. In Section 5 we discuss the
28 method by which this general formulation may be applied to a specific AM tech-
29 nology, in this case Selective Laser Sintering (SLS). Example results from two
30 SLS test problems are then given in Section 6. The concluding Section 7 presents
31 the discussion of the results achieved, methods for generalizing the present work

1 to AM technologies that are not powder based, and other advancements which
2 are necessary to further improve the DEM simulation methodology.

3 **2. Powder-Based Additive Manufacturing**

4 Powder-based additive manufacturing is based on the concept of fusing fine
5 granules of material using directed energy deposition. This is distinct from
6 processes such as stereolithography [9] or Fused Deposition Modeling (FDM)
7 [10] which use liquid or bulk solid feedstocks (respectively). Research towards
8 powder-based additive manufacturing dates back to the late 1970's [11], with
9 commercial processes and systems emerging in the late 1980's and early 1990's
10 [12]. Numerous processes have been developed, first using polymers and more
11 lately encompassing metals, ceramics, and other materials. Details on some of
12 the most common techniques currently in use are described below. Generally,
13 the standard terminology given by the ASTM standard 2792 [13] is employed
14 hereafter.

15 SLS is the oldest of the powder-based additive manufacturing technologies
16 and was developed in the late 1980's at the University of Texas [14]. This pro-
17 cess distributes a powder feedstock, usually a polymer, in a thin uniform layer
18 across the top surface of the build domain. A laser energy source is then used
19 to selectively fuse the powder via sintering. The build domain is lowered and
20 the process is repeated until the specified object has been completed. This pro-
21 cess typically occurs under an inert atmosphere in order to prevent oxidizing
22 reactions. Further details on SLS can be found in [15–17]. While SLS most com-
23 monly employs polymer feedstocks, metal powders are also used. In cases where
24 metals are used, the term Direct Metal Laser Sintering (DMLS) is commonly
25 employed.

26 DMLS is a direct descendant of SLS [18, 19] and varies from that process
27 only in the fine details which differentiate the bonding mechanisms of metals
28 and polymers [20]. Stainless steels [21], titanium alloys [22, 23], copper alloys
29 [24], nickel alloys [25], aluminum alloys [26], and various other materials have
30 been widely used with the DMLS process.

1 Selective Laser Melting (SLM) operates on a similar principle to SLS and
2 DMLS, but employs higher energy densities in order to selectively heat the
3 feedstock powder above the liquidus temperature [27]. By doing so, lower void
4 fractions and higher densities are achieved in manufactured components. How-
5 ever, because of the higher energy density and the complex behaviors of the
6 molten pool, control of the process is more difficult and deleterious phenomena
7 such as thermal stresses emerge [28]. Work in SLM has primarily been focused
8 on iron and steel feedstocks [29], but some work has been done with nickel
9 superalloys [30].

10 Electron Beam Melting (EBM), sometimes known as Selective Electron Beam
11 Melting (SEBM) is closely related to SLM. In EBM energy input is accomplished
12 by means of an electron beam, which is directed using magnetic lenses. Unlike
13 the technologies described previously, EBM occurs in a vacuum environment
14 and the feedstock materials are preheated to a greater extent. A comparative
15 review of EBM and SLM is offered by [31]. EBM permits the use of a very
16 broad range of materials; steels [32] and titanium [33] are common, but exotic
17 materials such as niobium [34] and beryllium have also fabricated by means of
18 EBM.

19 Direct Metal Deposition (DMD) [35, 36] and Laser Engineered Net Shap-
20 ing (LENS) [37, 38] are processes for powder-based manufacturing which differ
21 substantially from the examples given earlier. Instead of fusing stationary beds
22 of powder, DMD and LENS processes actively inject or “jet” the feedstock
23 material into a melt pool produced by a laser thus combining mass with en-
24 ergy deposition. Typically the laser optics and particle jet nozzles are mounted
25 concentrically on the end of a robotic manipulator. This allows for the con-
26 struction of very large components, as well as the deposition of material onto
27 existing components in repair applications [39].

28 The combination of processes and materials which are available using powder-
29 based additive manufacturing has led to widespread use of this technology across
30 many industries [7]. In both the case of powder bed methods such as SLS and
31 powder jet methods such as DMD it is clear that the mechanics of granular

1 systems play a large role in the AM process. A methodology well-suited for the
2 study of such systems is introduced in the next section.

3 **3. The Discrete Element Method**

4 The Discrete Element Method (DEM) is a numerical method for simu-
5 lating the behavior of both continuous and discontinuous material systems.
6 DEM simulations are based on the Newtonian interactions of a system of par-
7 ticles. These particles are imbued with constitutive behaviors including con-
8 tact/collision models, heat transfer models, the ability to form and break inter-
9 particle bonds, and respond to external fields. While first discussed in [40], a
10 modern general reference on the DEM can be found in [8]. Other, more applied,
11 overviews are given by [41, 42]. The interested reader will find that a great deal
12 of the research on the DEM is found in the geomechanics and rock mechanics
13 literature, owing to this method’s usefulness in problems of brittle fracture (e.g.
14 [43, 44]). Other common areas of application are the study of granular flows
15 [45], ball mills [46], and ballasts [47].

16 *3.1. Formulation*

17 A DEM simulation contains a number of abitrarily-shaped particles, a subset
18 of which may be “bonded,” or attached to each other. To the extent that
19 they contact each other both bonded and unbonded particles participate in
20 Newtonian collisions which produce reaction forces which in turn propagate
21 into changes in particle velocity and position. A schematic overview of the
22 associated concepts from the perspective of interacting particles is shown in
23 Figure 2. While this figure depicts spherical particles, it important to note that
24 this approximation is not generally applicable. Because contact stiffness is a
25 function of local curvature, and contacts between aspheric particles will result
26 in tangential and moment forces, this approximation must be applied with care.
27 The major conceptual elements of a general DEM implementation are as follows:

28 [Figure 2 about here.]

1 *1. Collision detection.* Generally, it is not practicable to exhaustively check
2 every particle in the DEM simulation for contact with all other particles; such
3 a search would be of $\mathcal{O}(n^2)$ complexity where n is the number of particles and
4 likely greater than 10^6 . For this reason, spatial subdivision schemes are used so
5 that collision searching is reduced to local neighborhoods. Common techniques
6 for spatial subdivision include grids [48], octrees [49], and heap sorting [50]. An
7 extensive review of collision detection techniques is given by [51].

8 *2. Inter-particle contact laws.* Once particles are determined to be in contact,
9 an appropriate contact relationship that captures the material constitutive re-
10 sponse must be applied. The most common form is a force-displacement rela-
11 tionship with both normal and shear terms, as shown in Figure 2. The simplest
12 formulation in terms of the normal ($\mathbf{f}_n$) and shear ($\mathbf{f}_s$) forces has the form

$$\mathbf{f}_n = k_n \delta \hat{\mathbf{x}}_n \quad (1)$$

13

$$\mathbf{f}_s = -\mu \|\mathbf{f}_n\| \frac{(\mathbf{v}_i - \mathbf{v}_j)}{\|\mathbf{v}_i - \mathbf{v}_j\|} \quad (2)$$

14 where k_n is a stiffness coefficient, μ is a friction coefficient, δ is the inter-
15 penetration distance defined in Figure 2 and $\mathbf{v}_i$, $\mathbf{v}_j$ are the velocity vectors
16 of the particles participating in the collision and $\hat{\mathbf{x}}_n$ is the unit normal vector
17 connecting the particle centers. Many more sophisticated contact models are
18 available and a summary of normal-force models can be found in [52], while
19 a discussion of shear-force models is given by [53]. Among the most frequent
20 augmentations made to the simple model of Equations (1-2) is the inclusion of
21 heat conduction.

22 *3. Boundary condition contact laws.* The interacting particles of the DEM
23 typically do not occupy an infinite unbounded space, therefore provisions for
24 boundary conditions must be made. The most common boundary conditions
25 are stationary and moving infinite planes. Testing particles for collision with
26 these planes is trivial and efficient. Periodic boundary conditions, e.g. those
27 employed in [54], are also common. For more complex cases, collision with

1 triangular meshes is commonly employed, using methods such as that given by
2 [48]. The contact laws applied are not necessarily the same as those for inter-
3 particle collisions, and may embody different constitutive behaviors than the
4 particle-particle case.

5 *4. Bond formation, deformation, and breakage.* An important feature of the
6 DEM is the formation of bonds between particles. This allows the simulation
7 of continuum domains and solid objects. Generally bonds are considered as
8 two or three-dimensional beams, which may support selected combinations of
9 axial, shear, and moment loadings. The use of bonds to capture the long-range
10 properties of materials is discussed in depth by [55]. Once formed, bonds deform
11 under mechanical forces, and break once a failure criterion is reached. This
12 allows the simulation of complex failure modes, such as delamination or fracture
13 [56], in a computationally efficient fashion. This topic is further examined by
14 [57].

15 *5. Time step integration.* Once the physical influences (e.g. forces, heat fluxes)
16 on every particle have been determined, it is necessary to propagate these in-
17 fluences motions of the particle system and step the DEM simulation forward
18 in time. An explicit Eulerian [58, 59] or Verlet [60, 61] time-step integration
19 is most widely used for this purpose. However, recent work has shown that
20 implicit methods are promising in this respect [59, 62].

21 *3.2. Related Methods*

22 The Discrete Element Method is only one of many particle-based methods
23 which find use in numeric simulations. One widely-used technique closely related
24 to the DEM is Molecular Dynamics (MD) simulation [63]. DEM and MD are
25 broadly similar methodologies, some researchers use the terms interchangeably
26 [64]. However, the DEM is distinct from MD formulations. It supports poly-
27 disperse particle systems, non-spherical particles, and particles with rotational
28 degrees of freedom; these features are not commonly found in MD implemen-
29 tations. We have selected DEM as the appropriate simulation methodology for

1 additive manufacturing exactly because of these features. In particular the fea-
2 ture of polydispersity makes DEM uniquely preferable due to the fact that it
3 enables accurate representation of feedstock powders that are characterized by
4 multiple particle size distributions.

5 Another widely used particle-like method is Smoothed Particle Hydrody-
6 namics (SPH) [65, 66], although in this case the term ‘hydrodynamics’ should
7 be read as ‘mechanics.’ In SPH, particles are augmented with a spatial ‘smooth-
8 ing length’ over which their properties are interpolated by a kernel function. A
9 comprehensive review of SPH may be found in [67]. SPH is most widely used
10 to simulate fluid mechanics [68], but has also been extended to the domain of
11 solids [69]. A thorough comparison of DEM, SPH, and MD methods is given by
12 [70]. Because powder-based additive manufacturing bears a much greater sim-
13 ilarity to the DEM formulation than SPH, we have concluded that employing
14 the former represents the most appropriate path forward. However, SPH may
15 be a valuable tool for simulating other AM technologies, especially when used
16 in a hybrid fashion with the DEM (e.g. the method of [71]).

17 3.3. DEM for Additive Manufacturing

18 The DEM has been widely employed to study granular systems [45, 53],
19 including pressure sintering [53]. However, it has not been employed to study
20 additive manufacturing processes to the same extent. One preliminary example
21 from the literature can be found in [72], however this example focuses on the
22 development of random packings, and does not investigate the physics of the
23 sintering process. From the discussion above it is clear that DEM has great
24 potential in this field. In the next section, we outline an algorithm which lever-
25 ages the well-suited formulation of the DEM to simulate powder-based additive
26 manufacturing in a physically realistic and computationally efficient fashion.

27 4. Methodology

28 Based on the review of powder-based additive manufacturing systems pre-
29 sented in the previous section, it is clear that DEM simulations of these pro-

1 cesses must perform several tasks in the most computationally efficient manner
2 achievable. These tasks are given in a general form below.

- 3 1. The DEM simulation must embody a system of particles with proper-
4 ties corresponding to the feedstock material for the AM process (either
5 polymer or metal). Both the mechanical and thermal responses of the
6 feedstock materials must be accurately modeled. The particle system it-
7 self must be expandable, in order to model continuous (as in the case of
8 DMD) or successive distinct (as in the case of SLS) additions of material
9 to the build domain over the course of the additive manufacturing process.
- 10 2. The boundary conditions of the simulation must define a domain mim-
11 icking that of the additive manufacturing process. In the case of AM
12 processes such as SLS, this ultimately requires the arrangement of parti-
13 cles into uniform flat layers.
- 14 3. The DEM simulation must apply heat energy to the particle system in such
15 a fashion that mimics the additive manufacturing process. In practice, the
16 simulation is required to read a computer numeric control (CNC) machine
17 code file, and position a heat source according to the directives of this code.
- 18 4. The particle system must react to the application of heat energy by form-
19 ing bonds, in order to model the consolidation process (sintering or melt-
20 ing) employed by the additive manufacturing technique.
- 21 5. An animated visual display of the particle system must be displayed to
22 the user of the simulation.

23 In order to accomplish these tasks, we developed a general DEM framework
24 for the simulation of additive manufacturing processes. The details regarding
25 different aspects of this framework, the constituent algorithms, and implemen-
26 tation are given in the sections below. Following this, in Section 5, the applica-
27 tion of this general framework to a particular additive manufacturing process is
28 given.

1 4.1. Particle System Definition

2 In this work we utilize a DEM particle system of N spherical particles oc-
 3 cupying a build domain $\Omega \in \mathbb{R}^3$ with a boundary Γ , with Cartesian spatial
 4 components (x, y, z) . The vector representing the centroid of particle i within
 5 Ω is denoted $\mathbf{p}_i$ and the corresponding vectors of particle velocity, acceleration,
 6 and force are denoted $\mathbf{v}_i$, $\mathbf{a}_i$, and $\mathbf{f}_i$ (respectively). The particle mass is m_i , its
 7 radius is r_i , while the temperature is represented by T_i , and the heat flux by q_i .
 8 A bond between any pair of particles i and j is represented by the tuple B_{ij} .

9 In the present work we define Ω to be a regular parallelepiped bounded such
 10 that $x_{min} \leq x \leq x_{max}$, $y_{min} \leq y \leq y_{max}$, and $0 \leq z \leq z_{max}$. We consider the
 11 gravity to act in the $-z$ direction with a magnitude of 9.81 m/s^2 . This domain
 12 is demonstrated in Figure 3.

13 [Figure 3 about here.]

14 The simulation time variable is t , with $t = 0$ corresponding to the introduc-
 15 tion of the first particles into Ω . The discrete simulation time step is Δt , and
 16 n_t is the total number of such time steps in the simulation. For stability, we
 17 demand $\Delta t \ll \Delta t_{crit}$, which is a critical time step determined from the particle
 18 system stiffness. A satisfactory approximation of the critical time step is given
 19 by

$$\Delta t_{crit} \simeq \sqrt{\frac{m_{min}}{k_n}} \quad (3)$$

20 where m_{min} is the minimum particle mass and k_n is the normal stiffness par-
 21 ameter of the particles from Equation 1. In most cases, satisfactory efficiency
 22 can be achieved simply by taking $\Delta t = \Delta t_{crit}/10$. More advanced schemes for
 23 determining this parameter, such as those given by [58, 59], may be employed
 24 in the future.

25 4.2. Spatial Searching and Collision Detection

26 A cursory analysis of powdered metals available, for example, for SLS addi-
 27 tive manufacturing shows that these powders are relatively fine, with particle
 28 diameters below 100 microns. As a result very large numbers of particles are

1 required to model even small additive manufactured objects; on the order of
 2 10^7 particles are required per cubic centimeter of build volume. Additionally,
 3 the particle system is highly polydisperse, and contains particles of different
 4 sizes. Both of these factors necessitate the use of an efficient collision detection
 5 algorithm.

6 Because of the polydispersity of the particle system, where the ratio of max-
 7 imum particle size to minimum particle size exceeds ten, we subdivide the
 8 collision detection problem into two parts termed ‘fine’ and ‘coarse’ detection.
 9 The coarse detection uses an octree spatial partitioning scheme similar to that
 10 described by [49]. For each particle location $\mathbf{p}_i$ the octree is queried to find the
 11 indices of the local subset E_i of particles

$$E_i = \{j : \|\mathbf{p}_i - \mathbf{p}_j\| \leq d_i\} \quad (4)$$

12 where d_i is the critical collision radius. In general, this is a conservative over-
 13 estimate of the size of the region which a particle occupies, plus a similar over-
 14 estimate of the region which another particle occupies. Here, we introduce the
 15 assumption that the DEM particles are spherical; based on existing micrographic
 16 studies of AM powders [29, 73–75], which show photograph of these powders
 17 under very high magnification, this is a reasonable approximation. This reduces
 18 the calculation of d_i to

$$d_i = r_i + \max(r_j, j = 1 \dots N) \quad (5)$$

19 To avoid excessive computations, the maximal particle radius is precomputed;
 20 when particles are added to or removed from the particle system this value is
 21 updated.

22 After coarse collision checking E_i contains all the indices of the particles that
 23 are tentatively in contact with particle $\mathbf{p}_i$. Furthermote, we perform refined
 24 collision checking within this vector of potential collisions and we construct the
 25 subset E'_i that contains the indices of the particles that are actually in collision
 26 with particle $\mathbf{p}_i$, according to

$$E'_i = \left\{ E_i^j : \|\mathbf{p}_i - \mathbf{p}_{E_i^j}\| \leq r_i + r_{E_i^j} \right\}. \quad (6)$$

1 It is computed by sequentially calculating the Euclidean norm-distance between
2 particles i and all members of E_i . As per Equation (4), E_i^j denotes the index of
3 particle j that was found to be in the coarse neighborhood of i . In cases where a
4 collision is found, the particle overlap δ_{ij} between particles i and j is computed
5 for use in the contact model.

6 4.3. Contact Modelling

7 Because of the many collision models available [52, 53] we adopt a general
8 approach to the computation of the contact force. Without loss of generality
9 we consider the normal and shear forces on particle i generated by contact with
10 particle j to have the form

$$f_{n_{ij}} = \phi(\mathbf{p}_i, \mathbf{v}_i, \mathbf{v}_j, T_i, \delta_{ij}) \quad (7)$$

$$f_{s_{ij}} = \zeta(\mathbf{p}_i, \mathbf{v}_i, \mathbf{v}_j, T_i, f_{n_{ij}}) \quad (8)$$

12 where ϕ and ζ are arbitrary functions. While this form encompasses many
13 common contact models such as Hertzian contact, or that of Equations (1-2),
14 it does not permit the use of the time-history of the particle positions or other
15 associated quantities. Because of the number of particles in the DEM simulation,
16 storing these time histories is relatively expensive. If a particular application is
17 found which requires these histories, further work will be necessary to determine
18 the most efficient implementation. Once Equations (6-7) have been evaluated
19 for every element of E_i' , the total force on particle i is computed

$$\mathbf{f}_i = \sum_{j=1}^{n_\epsilon} [f_{n_{ij}} + f_{s_{ij}}] + \sum_{j=1}^{n_B} f_{B_{ij}} - c_d \mathbf{v}_i - m_i \mathbf{g} \quad (9)$$

20 where n_ϵ is the number of contacts, n_B is the number of bonds, c_d is a viscous
21 drag coefficient and $\mathbf{g}$ is the gravity vector. The computation of the bond forces
22 $f_{B_{ij}}$ is discussed in Section 4.6.

23 In addition to the generation of mechanical forces, particle collisions also
24 result in the transfer of heat energy. We model this transfer as pure conduction,
25 and neglect radiative or convective effects between particles. Therefore the heat

1 flux on particle i from particle j is computed by

$$q_{ij} = k_t (T_j - T_i) \quad (10)$$

2 where k_t is a heat conduction coefficient which necessarily depends on the phys-
 3 ical properties and size of the powder particles, as well as the inter-particle con-
 4 tact cross-sectional area (and thus $\mathbf{f}_n$). This coefficient may also be dependent
 5 upon on the particle temperature. The total heat flux on particle i is simply

$$q_i = \sum_{j=1}^{n_e} q_{ij} \quad (11)$$

6 The formulation presented in Equations (8) and (10) neglects the effects of
 7 boundary conditions, which are addressed in the next section.

8 4.4. Boundary Conditions

9 In this work we employ planar spatial boundary conditions. These planar
 10 boundary conditions may be infinite, half-infinite, or fully bounded in size. Ad-
 11 ditionally, these planes may be stationary, or move over time. The particle-plane
 12 collision detection of [51] is used. Because of the limited role played by spatial
 13 boundary conditions in the AM process we do not imbue them with a sophisti-
 14 cated material model. If particle i impinges on bounding plane k defined by a
 15 unit normal vector $\mathbf{n}_k$, it experiences a normal to the plane force

$$\mathbf{f}_{bn_{i,k}} = k_b (r_i - \delta_b) \mathbf{n}_k \quad (12)$$

16 where k_b is the boundary stiffness parameter and δ_b is the minimal distance
 17 between the particle i and the bounding plane k . From this normal force, a
 18 shear force is also computed by

$$\mathbf{f}_{bs_{i,k}} = \mu_b \|\mathbf{f}_{bn_{i,k}}\| \bar{\mathbf{v}}_i \quad (13)$$

19 where μ_b is the boundary friction coefficient and $\bar{\mathbf{v}}_i$ is the particle velocity
 20 projected onto the bounding plane. In addition to these mechanical forces, the
 21 planar boundary conditions also participate in heat transfer. If a particle is in
 22 contact with a bounding plane, its heat flux is adjusted

$$q_{i+} = k_{tb} (\tau_e - T_i) \quad (14)$$

1 with k_{tb} corresponding to the heat conduction coefficient for the boundary and
 2 τ_e is the the ‘environment’ or process background temperature. Typically, we
 3 take $k_{tb} = k_t$. For the most part the planar boundary conditions serve to dissi-
 4 pate heat energy, which is introduced into the particle system by a concentrated
 5 source. This is discussed in the next section.

6 4.5. Energy Application

7 The advantageous aspects of additive manufacturing are derived from the
 8 highly directed manner in which energy is transferred to the raw feedstock
 9 material. In powder-based additive manufacturing systems this is achieved by
 10 means of a laser or electron beam, the position and orientation of which is
 11 guided by a computer-controlled mechatronic device. The geometric complexity
 12 observed in existing additive manufacturing processes dictates that the pattern
 13 of heat deposition into the feedstock powder will be highly non-uniform in terms
 14 of both the spatial and temporal variables.

15 In physical additive manufacturing systems, the movement of the heat source
 16 that defines the deposition paths, is dictated by a series of numeric control (NC)
 17 directives, often collectively known as ‘G-code.’ While G-code is a specific NC
 18 programming language, the term is often used in a general sense to refer to
 19 any NC program. In practice, the NC code varies substantially in composition
 20 between AM technologies, and between AM hardware manufacturers. In the
 21 DEM simulation, this NC code is read and interpreted in order to capture the
 22 motion of the laser (or e-beam) heat source. The specifics of this interpretation
 23 vary between AM technologies; independent interpreters are needed for specific
 24 processes. The output of the interpreter is a function of time which outputs
 25 the spatial coordinate of the laser, denoted $\gamma(t)$. This function has a piecewise-
 26 continuous form

$$\gamma(t) = \begin{cases} \gamma_0(t), & 0 \leq t < t_0 \\ \gamma_1(t), & t_0 \leq t < t_1 \\ \vdots & \\ \gamma_n(t), & t_{n-1} \leq t < t_n \end{cases} \quad (15)$$

1 where each of the γ_n components corresponds to a straight-line, circular, or
 2 elliptical motion of the heat source. During the initialization of the DEM sim-
 3 ulation, $\gamma(t)$ is uniformly sampled

$$P = \{\gamma(0), \gamma(\Delta t), \gamma(2\Delta t), \dots, \gamma(n\Delta t)\} \quad (16)$$

4 For periods of time in which the laser turned off, e.g. when powder is being
 5 distributed in SLS processes, P is constructed to return a value which signals
 6 the DEM simulation to skip the steps described in the next paragraph.

7 The above procedure is a pre-processing step which is performed before the
 8 DEM simulation begins. Therefore, the position of the heat source is known
 9 at every time step, this information is contained in P . With this information,
 10 there are many models which may be employed to compute the heat energy
 11 transferred to the particles proximal to this location. Some recent examples of
 12 such models are presented in [76]. In our DEM implementation the zone of heat
 13 input is bounded by a sphere of finite radius r_e . At every time step ($t = n_t\Delta t$),
 14 after collision and boundary processing, the distance between each particle and
 15 $\gamma_{n_t} = \gamma(n_t\Delta t)$ is computed. If this distance is less than r_e additional heat flux
 16 is applied according to

$$\mathbf{q}_i = \begin{cases} \lambda(\|\mathbf{p}_i - \gamma_{n_t}\|), & 0 \leq \|\mathbf{p}_i - \gamma_{n_t}\| \leq r_e \\ 0, & otherwise \end{cases} \quad (17)$$

17 where λ is a symmetric function describing the distribution of heat flux within
 18 the sphere. Typical constructions for λ include constant heat flux, or a Gaussian
 19 distribution. Figure 4 demonstrates the methodology for energy application in
 20 a notional fashion.

21 [Figure 4 about here.]

22 4.6. Sintering and Bond Formation

23 From a data-management perspective, the most complex aspect of the DEM
 24 simulation is the collection of procedures associated with inter-particle bonding.
 25 This is because, in contrast to the constitutive contact laws, the bonds are

1 defined upon pairs of particles. These pair-wise constitutive behaviors must
 2 capture the formation of bonds, store them, compute their response to thermo-
 3 mechanical (and perhaps other) loadings, and finally account for cases of bond
 4 failure.

5 The bond formation process is integrated with the contact detection scheme
 6 described earlier. If particles i and j are in contact, that is if $j \in E'_i$, a set of
 7 bonding criteria are evaluated after the computation of normal and shear forces.
 8 The criterion includes a condition for sufficient temperature

$$T_i \geq \tau_s \text{ and } T_j \geq \tau_s \quad (18)$$

9 where τ_s is the critical sintering temperature, a condition for sufficient contact
 10 pressure

$$\|\mathbf{f}_{nij}\| \leq f_{crit} \quad (19)$$

11 where f_{crit} is the critical contact compressive force, and a condition for suffi-
 12 ciently small relative velocity

$$\mathbf{v}_i \cdot \mathbf{v}_j \leq v_{crit} \quad (20)$$

13 where v_{crit} is the critical relative velocity. As a result of this simple pair-wise
 14 local bonding a complex network of bonds rapidly arises in the DEM simulation,
 15 trailing the path of the directed energy application. A two-dimensional example
 16 of this process is shown in Figure 5.

17 [Figure 5 about here.]

18 Storing and managing the structure of bonds in the DEM simulation is equiv-
 19 alent to the problem of graph adjacency, as described by [77], with the DEM
 20 particles being analogous to graph vertices and inter-particle bonds analogous
 21 to graph edges. Due to the size of the DEM particle system, and the sparse
 22 localized nature of the bonding process, we employ an adjacency list approach
 23 to storing the bonds. The particle centroids $\mathbf{p}_i$ are used as a vertex list V ,
 24 which is augmented by an adjacency list B . This list is structured such that
 25 each element B_i is itself a list of vectors. Each of these vectors, denoted B_{ij} ,

1 corresponds to the j^{th} inter-particle bond associated with particle i . In the
 2 present work we use the form

$$B_{ij} = \{k, \delta_0, k_B, \varepsilon_\infty\} \quad (21)$$

3 where k is the index of the particle with which i is bonded, δ_0 is the initial bond
 4 length, k_B is the bond stiffness, and ε_∞ is the bond failure strain. In general
 5 the last two parameters have the form

$$k_B = \theta(T_i, T_k, \mathbf{f}_{n_{i,k}}) \quad (22)$$

$$\varepsilon_\infty = \eta(T_i, T_k, \mathbf{f}_{n_{i,k}}) \quad (23)$$

7 where θ and η are functions chosen to capture the effects of contact pressure
 8 and temperature on the sintering process.

9 At every time step each bond is evaluated in one of two ways. If $T_i \geq \tau_s$
 10 then the bonds do not exert a mechanical force on particle i . Instead, the bond
 11 properties of B_{ij} are recomputed using the conditions of the current time step.
 12 If $T_i < \tau_s$, then for every bond on particle i exerts a force

$$f_{B_{ij}} = k_B (\|\mathbf{p}_i - \mathbf{p}_j\| - \delta_0) \quad (24)$$

13 where k_B and δ_0 are taken from B_{ij} . It is important to note that, because differ-
 14 ent bonds will possess different coefficients, simple bond constitutive behaviors
 15 may produce long-range anisotropic responses in the bonded DEM particle sys-
 16 tem. When a bond reaches the failure strain

$$\left| \frac{\|\mathbf{p}_i - \mathbf{p}_j\| - \delta_0}{\delta_0} \right| > \varepsilon_\infty \quad (25)$$

17 it is assumed to fail cleanly and instantaneously. The corresponding entry in B_i
 18 is deleted and the bond ceases to exist on all subsequent time steps.

19 4.7. Time Step Integration

20 While a number of different time-step integration schemes have been devel-
 21 oped for the DEM [58], in this work we use the common Euler explicit integration
 22 method. While Verlet integration is generally superior in DEM applications, we

1 use the Euler algorithm to demonstrate the functionality of the DEM in the
2 context of additive manufacturing even using a minimal implementation of ba-
3 sic algorithms. At every time step, after the forces and heat fluxes have been
4 calculated in the fashion outlined above, we apply the update scheme expressed
5 by

$$\mathbf{v}_i^{t+\Delta t} = \mathbf{v}_i^t + \frac{\mathbf{f}_i^t}{m_i} \Delta t \quad (26)$$

$$\mathbf{p}_i^{t+\Delta t} = \mathbf{p}_i^t + \mathbf{v}_i^t \Delta t \quad (27)$$

7 to update the particle positions and velocities, and

$$T_i^{t+\Delta t} = T_i^t + \frac{q_i^t}{m_i} \Delta t \quad (28)$$

8 to update the temperatures.

9 4.8. Visualization and Post-Processing

10 In order to develop, debug, calibrate, and use a DEM simulation it is almost
11 mandatory to provide a visual depiction of the particle system to the program-
12 mer or user. This is a demanding task, as a typical additive manufacturing DEM
13 simulation involves millions or more particles. Additionally, using conventional
14 techniques, each particle must be displayed as a set of hundreds or thousands
15 of polygonal faces. Despite the power of modern computer graphics processors,
16 it is not practical to display these DEM systems in this fashion. In order to
17 achieve a “real-time” visualization, where the rendering time $t_{vis} \ll \Delta t$, we
18 adopt an approach commonly employed in the early days of computer graphics
19 when processing resources were much more scarce.

20 We utilize an approach known as “billboarding,” which is described in depth
21 by [78]. For each particle, a rectangular billboard of two triangles with a shared
22 hypotenuse is computed. The center of this billboard is located at $\mathbf{p}_i$, and it
23 is oriented such the billboard is normal to the view vector (the vector from the
24 simulation view point to $\mathbf{p}_i$). Since the particles are presumed to be spherical,
25 a circle may be drawn on this billboard to emulate a sphere. The area outside
26 of the circle is discarded, so as not to obscure other particle billboards. This

1 technique enables the display of tens of millions of particles at a frame rate
2 adequate for interactive graphics.

3 *4.9. Implementation*

4 The procedures outlined in the previous sections were implemented in the
5 C++ programming language. The flow of execution in this implementation is
6 shown in Figure 6. Notably, it can be seen that the calculations laid out earlier
7 are well-suited to parallel processing [79]. In this case we utilize the OpenMP
8 shared-memory parallel programming framework [80] to parallelize the inner-
9 most program loop which applies the calculations given earlier to each particle.
10 In order to provide a graphical user interface (GUI) we make use of the Qt
11 cross-platform application framework [81]. Qt’s signal/slot mechanism is also
12 used for communication between the DEM computation thread and the graphics
13 thread. In addition to the display of the particle system, this framework allows
14 for basic user interaction functions, such as file dialogs, adjusting the simulation
15 view point, and issuing start/stop commands to the particle system simulation.

16 [Figure 6 about here.]

17 **5. Application to Laser Sintering**

18 The formulation given in the previous section is very general, and can be
19 applied to any powder-based additive manufacturing technology. In this sec-
20 tion, we demonstrate the steps necessary to apply the methodology to Selective
21 Laser Sintering (SLS). We selected this methodology because of its commercial
22 prominence and because it requires the most sophistication in terms of bound-
23 ary conditions. There are five major steps which must be taken in order to
24 apply the DEM methodology to the SLS Process:

- 25 1. Determination of feedstock powder characteristics and properties.
- 26 2. Selection of particle constitutive equations.
- 27 3. Selection of DEM parameters.
- 28 4. Development of appropriate spatial boundary conditions.

5. Computation of appropriate energy application G-code.

Each of these steps is given in detail in the following sections.

5.1. Feedstock Powder Characteristics

For this application, we chose to study 316L stainless steel, which is widely used in SLS additive manufacturing. It is also beneficial that the mechanical properties of the bulk material are very well understood. Previous work [82] has experimentally measured the size distribution of 316L powders intended for use in AM applications. However, because of the bounded nature of particle size we do not entirely agree with the conclusions of [82], particularly the use of a Gaussian distribution to characterize the particle size variation. We extracted the numeric size data from this earlier work, and re-fit Weibull distributions to characterize the variations in particle shape. These data are shown graphically in Figure 7 and numerically in Table 1. Of these three samples, we selected $S2$ to govern our DEM particle system. Therefore the particle radii are randomly generated from a Weibull distribution with $k = 3.55$ and $\lambda = 31.4$.

[Figure 7 about here.]

[Table 1 about here.]

In addition to the particle size distribution, the physical properties of 316L stainless steel are also required. In this case we draw all values for physical properties from [83]. From these physical properties, the parameters defined in the previous section may be calculated. Before these calculations can be performed, it is necessary to select the exact form of the constitutive equations governing the particle interactions.

5.2. Constitutive Equation Selection

The DEM defined in Section 4 embodies the constitutive response of the particle system as four equations: ϕ , ζ , θ , and η . These functions capture the normal contact force, shear contact force, bond force, and bond failure strain (respectively). Because the present work is exploratory in nature, and

1 primarily intended to establish the DEM framework for AM problems in general
 2 as opposed to rigorously study one particular material system, we choose simple
 3 forms for these constitutive equations. We select

$$\phi(\mathbf{p}_i, \mathbf{v}_i, \mathbf{v}_j, T_i, \delta) = \phi(\delta) = k_n \delta \quad (29)$$

4

$$\zeta(\mathbf{p}_i, \mathbf{v}_i, \mathbf{v}_j, T_i, \mathbf{f}_n) = \zeta(\mathbf{f}_n) = -\mu \|\mathbf{f}_n\| \frac{\mathbf{v}_i - \mathbf{v}_j}{\|\mathbf{v}_i - \mathbf{v}_j\|} \quad (30)$$

5 to model the particle contacts, as shown in Figure 2. A constant value is chosen
 6 for both the particle-particle bond stiffness, and the bond failure strain. The
 7 bond stiffness is set equal to the particle contact stiffness,

$$k_B = k_n \quad (31)$$

8 and the bond failure strain is

$$\varepsilon_\infty = 0.4 \quad (32)$$

9 At present, we focus mainly on the additive manufacturing process, and we
 10 observe that this failure point is never reached by bonds in the particle system.
 11 In the future, when the AM components are subjected to mechanical load, this
 12 failure point will be of greater importance. To model the laser heating of the
 13 powder bed, we take

$$\lambda(\|\mathbf{p}_i - \gamma_{nt}\|) = Q \frac{r_i^3}{r_e^3} \quad (33)$$

14 Where Q is the total laser power distributed amongst the particles upon which
 15 it impinges in a spatially uniform, volumetrically proportional fashion.

16 5.3. Parameter Selection

17 The formulation of the previous section involves a number of physical con-
 18 stants, and parameters derived from documented physical constants resources.
 19 For completeness, Table 2 enumerates the numeric values for all of the DEM sim-
 20 ulation parameters used. Notably, the Hertz-Mindlin model is used to compute
 21 the normal stiffness, as detailed by [84], and the thermal conduction coefficient
 22 is calculated by

$$k_t = \frac{S\Lambda}{2\bar{r}c_p} \quad (34)$$

1 where S is the heat transfer surface area $\pi\bar{r}^2$, Λ is the material’s heat conductiv-
2 ity, $\bar{r}$ is the average particle radius, and c_p is the material’s heat capacity. Values
3 for the laser properties were derived from a cursory overview of commercially
4 available SLS systems.

5 [Table 2 about here.]

6 The value of the drag coefficient c_d is not derived from the physical proper-
7 ties of the additive manufacturing system, environment, or materials. Rather,
8 it is a non-physical parameter used to dissipate kinetic energy imparted to the
9 particles by both gravitation and the scraper boundary condition. Its value was
10 set at the smallest value that produced an equilibrated powder bed within the
11 allotted settling time. We justify this non-physical damping term by noting that
12 the particle system is allowed to equilibrate to a state of effectively zero ki-
13 netic energy before application of the laser heat source. This implies that the
14 parameters affecting the free-body motion of the particles will not directly af-
15 fect the bond-forming sintering process, and will thus not affect the geometry
16 of the bonded particle system. However, this non-physical coefficient should be
17 viewed with caution, and in future implementations constitutive relationships
18 that dissipate energy in a more physically realistic manner should be considered.

19

20 5.4. Mechanical Boundary Conditions

21 The purpose of the planar mechanical boundary conditions is to re-create
22 the mechanical processes by which the deposition of uniform layers of feedstock
23 powder is accomplished in a physical SLS machine. We are not concerned with
24 the free granular dynamics of the particles before their entry into the build
25 domain, and therefore do not simulate some aspects of the powder-handling
26 machinery. The methodology employed is to generate a uniform grid of particles
27 (with small perturbations in position), and allow these particles to drop a slight
28 distance into the build domain. This allows the gravitational force to loosely
29 compact the particles into a layer, but does not produce the uniform surface
30 required for additive manufacturing.

Once the powder particles have been deposited into the build domain, moving boundary conditions are used to compact them into a uniform bed. We experimented with several combinations of boundary conditions for this purpose, such as static or vibrating planes which moved along the z -axis in order to achieve compaction. Of these methods, the best performance was achieved using a “scraper” arrangement which closely mimics the physical additive manufacturing process. The scraper boundary conditions are illustrated in Figure 8.

[Figure 8 about here.]

The angled segment of the stationary boundary conditions in Figure 8 is a convenient means to prevent discontinuous application of force to the particle by the boundary conditions. Similarly, the speed of the moving boundary conditions must be restricted in order to prevent destabilization of the explicit time stepping scheme. The results of the simulation are not sensitive to the value chosen for this velocity, in most cases we take the scraper to move at a rate of 10-20 mm/s .

17 *5.5. Geometry and Slicing*

In order to simulate the SLS process, it is necessary to convert the digital representation of the object to be produced into a sequence of laser heat-source movements, as described in Section 4. In practice, this is accomplished by a software tool known as a “slicer”, which typically takes a triangulated stereolithography (STL) file as input. The topic of slicing algorithms is reviewed by [85, 86]. Slicing is a demanding geometrical computation with many details and special cases which must be implemented for specific AM technologies, and even specific AM machines. Broadly speaking, the slicer operates by intersecting the STL model with a series of planes in order to define a series of cross sections. For each of these planes, both perimeter and infill trajectories are computed in order to produce a layer.

While several commercial solutions for slicing in the domain of metal SLS additive manufacturing are available, they operate in close connection with the

1 AM hardware and we were unable to utilize these tools for the present research.
2 Therefore we implemented a simple slicing algorithm which replicated the basic
3 behaviors which we observed in commercial tools. This slicer takes as input the
4 STL model, and parameters for total model height (h), layer thickness (Δh), and
5 laser beam radius (r_e). It then intersects the STL model, which consists only
6 of a set of triangular facets, with a series of planes parallel to the z -axis spaced
7 at intervals of Δh . For each layer, this results in a set of closed piecewise-linear
8 curves. For each closed curve, three laser trajectories are computed:

- 9 1. A trajectory tracing the closed curve exactly - the “outer perimeter.”
- 10 2. A trajectory inset from the first by $2r_e$ - the “inner perimeter.”
- 11 3. A uniform raster pattern with spacing of $2r_e$ which fills the interior of the
12 inner perimeter - the “infill.” The raster pattern is rotated by 90° degrees
13 between layers.

14 A demonstration of this simple slicer is given in Figure 9. Each of the three
15 paths listed above are uniformly sampled at equal increments corresponding to
16 a given laser velocity (v_l) in order to produce the laser NC code. Once the laser
17 NC codes for each layer have been produced, they are interleaved with separate
18 commands for the simulation to perform other functions. These include actions
19 such as depositing particles, advancing the scraper boundary conditions, and
20 enforcing a cool-down time after the laser sintering of each layer. This produces a
21 coherent sequence of events which allow the simulated production of the original
22 STL model using the DEM particle system.

23 [Figure 9 about here.]

24 6. Results

25 In order to demonstrate the general methodology of Section 4, coupled with
26 the specific methodology for SLS of Section 5, we conducted a pair of test
27 simulations. In both cases the DEM methodology was used to simulate the SLS
28 construction of a different input geometric model. The first test model is the

1 well-known “Stanford Bunny,” while the second is a small jet turbine blade.
2 In both cases the computing platform employed was a workstation computer,
3 with dual six-core processors operating at 2.0 GHz and 128 GB memory. We
4 note that the DEM simulations did not require such a large amount of memory,
5 typically less than one GB was required.

6 6.1. Test Case 1: Stanford Bunny

7 The first test case utilized a low-polygon interpretation of the well-known
8 “Stanford Bunny” model. The input STL model, and the resultant G-code
9 paths, are shown in Figure 10. The parameters utilized by the slicer are given
10 in Table 3.

11 [Figure 10 about here.]

12 [Table 3 about here.]

13 Several snapshots of the first layer of the DEM simulation can be seen in Fig-
14 ure 11. Snapshots at the completion of several layers, throughout the DEM
15 simulation, are shown in Figure 12. In this figure, the intermediate layers were
16 chosen to show the more irregularly-shaped cross sections of the model while
17 under construction.

18 [Figure 11 about here.]

19 [Figure 12 about here.]

20 A comparison of the final DEM output to the original input model is pre-
21 sented in Figure 13. The output model shown in this figure was computed
22 by performing a Poisson-surface reconstruction [87] of the set of points defined
23 by centroids of all particles which were bonded to at least one other particle,
24 $\{i : B_i \neq \{\}\}$. Inspection of the final portion of Figure 12 and the comparison
25 shown in Figure 13 allows some insight into the behavior of the DEM simula-
26 tion. It is clear that the DEM simulation of the SLS process recreates the basic
27 geometry of the input model. This is not a perfect translation, and several

1 defects can be seen in the output DEM model. In Figure 12 the “stair-step”
2 phenomenon can be clearly seen; this is a well known artifact produced by SLS
3 and other AM systems. Additionally, some loss of definition in the output model
4 is present; for instance the sharp facet edges of the STL model are not seen in
5 the output. This is caused primarily by two factors; the small size of the input
6 model $h = 2mm$ and the high rate of heat deposition. The model height is near
7 the lower limit permissible for most commercial systems. This causes particles
8 outside of the domain of the input model to reach temperatures high enough
9 for sintering. Consequently, this promotes the formation of extraneous bumps,
10 as can be seen in several locations on the output model.

11 [Figure 13 about here.]

12 6.2. Test Case 2: Turbine Blade

13 While the first test case focused on a well known, but non-functional geom-
14 etry, the second test case used the geometry of a small jet turbine blade. The
15 input STL model, and the resultant G-code paths, are shown in Figure 14. The
16 parameters utilized by the slicer are given in Table 4. These parameters are
17 the same as those used in the previous test case, except for the laser power.
18 This has been reduced by a factor of two in order to improve the fidelity of the
19 output DEM model. Additionally, it should be noted that the laser velocity is
20 kept constant, which combined with an input model much larger in size results
21 in a lower power density delivered to the particle system over time.

22 [Figure 14 about here.]

23 [Table 4 about here.]

24 Several snapshots of the one layer of the DEM simulation can be seen in Fig-
25 ure 15. As the first layer is a plain rectangle, the snapshots shown are from a
26 layer where the turbine airfoil is beginning to emerge. Snapshots at the comple-
27 tion of several layers, throughout the DEM simulation, are shown in Figure 16.
28 As before, the intermediate layers were chosen to show interesting non-uniform

1 sections of the model while under construction. Additionally, the visualization
2 portion of the DEM code was modified so as to not render unbonded particles
3 which were deeply buried in the particle system; this allows a more adequate
4 “live” view of the simulation, which in turn allows the user to monitor develop-
5 ments more clearly.

6 [Figure 15 about here.]

7 [Figure 16 about here.]

8 Finally, a comparison of the DEM output to the original turbine blade model
9 is presented in Figure 17. Here, we see that the thermally induced inaccuracies
10 are smaller, especially examining the lower dovetailed portion of Figure 15 where
11 the stair-step area is located. Some surface irregularity is present, and as before
12 the stair-step effect is clearly present. The broad curved surfaces of the turbine
13 blade exhibit small-scale bumpiness, the source of which is clear when frame
14 three of Figure 15 is examined. The raster heat pattern is producing higher
15 heat densities at the edges of the airfoil surface, which in turn promotes the
16 accumulation of small bumps and irregularities. When the results of Figures
17 15-17 are viewed together, however, it is clear that the DEM simulation of the
18 SLS process has produced a result of high geometric fidelity.

19 [Figure 17 about here.]

20 *6.3. Computational Performance*

21 The simulation results presented in the previous sections are notable because,
22 despite the modest computing resources employed, they did not require excessive
23 computation time. Table 5 presents the size and computing time required for
24 the test problems.

25 [Table 5 about here.]

26 The bulk timing figures of Table 5 can be broken down into the time required
27 to re-build the octree data structure and the time required for the DEM com-
28 putation. In both test cases rebuilding the octree at the beginning of each time

1 step required approximately 14% of the total time consumed. Of the remaining
2 DEM computing time, more that 91% is spent by the collision-detection algo-
3 rithm, with the vast majority of this going to the octree search. The remaining
4 9% is dominated by the calculation of particle collision forces and evaluating
5 bond formation. The above mentioned figures refer to a single thread of execu-
6 tion. The collision detection and force/bond formation algorithms are inherently
7 parallelizable and our tests show almost linear scaling with number of threads
8 of execution. It should be noted that the octree rebuild algorithm was not par-
9 allelized.

10 The scaling from the small to the large example is caused by both slowdown
11 in the DEM computation loop (due to the increased number of particles) and
12 due to the longer timespan which must be simulated. The total time period
13 simulated in the turbine blade problem is approximately five times the one re-
14 quired for the Stanford Bunny problem. Given that the ratio of simulation time
15 is roughly 1:5 and the ratio of number of particles is roughly 1:10 the compu-
16 tation time ratio of 1:55 indicates that the DEM implementation is exhibiting
17 reasonable performance scaling.

18 **7. Conclusions**

19 In this work, we have developed a DEM framework for the analysis of
20 particle-based additive manufacturing technologies. This formulation allows
21 us to express the constitutive behaviors of the DEM particles and bonds as a
22 small set of equations and parameters, which may be suitably adapted to a wide
23 range of processes. We have demonstrated the adaptation of this framework by
24 application to a specific additive manufacturing process (SLS), and by further
25 applying this simulated process to a pair of test components. The test results
26 of Section 6 demonstrate that this simulation framework is capable of captur-
27 ing the spatially and temporally varying distributions of heat and mechanical
28 forces within the additively manufactured object. It is seen that the results
29 of the DEM simulations replicate their input geometries, while also exhibiting

1 features which are characteristic of the physical additive manufacturing pro-
2 cess which is simulated. Additionally, the timing results of Section 6 show that
3 the additive manufacture of specimens of sufficient size for physical testing is
4 feasible within a modest computational budget.

5 The present work is exploratory in nature, and our primary intent has been
6 to provide a framework for future detailed studies of additive manufacturing
7 materials, processes, and components. As a result, the models chosen and
8 assumptions made in order to simulate the SLS process and 316L stainless
9 steel feedstock are simplistic in nature. Additionally, there are a wide range of
10 powder-based additive manufacturing feedstock materials and processes, which
11 differ significantly from SLS. Finally, the present work does not encompass the
12 post production loads and fields to which additively manufactured components
13 are subjected. Clearly there are several important development and extensions
14 of the present work which are both valuable and feasible from a technical per-
15 spective. It is anticipated that the three most important near-term extensions of
16 the present work are:

- 17 1. Developing and implementing more realistic particle and bond constitutive
18 models for the 316L material system.
- 19 2. Developing the boundary condition formulations required for applying
20 multi-physics loads to the bonded particle systems produced by the addi-
21 tive manufacturing process simulation.
- 22 3. Developing DEM framework extensions that will enable its implemen-
23 tation for other additive manufacturing technologies such as particle-jet
24 methods.

25 As part of our planned near-term future work, a Verlet or velocity-Verlet inte-
26 gration algorithm will be employed due to its inherently superior stability and
27 performance. Additionally, a software implementation that utilizes distributed
28 memory parallelization is anticipated to be important for the simulation of larger
29 build volumes.

30 In addition there are several longer term extensions of the present work

1 which may be of value, but will require more significant adaptation of the DEM
 2 methodology. One such extension is the study of Fused Deposition Modeling
 3 (FDM) additive manufacturing processes [88]. These thermoplastic extrusion
 4 methods differ substantially from those mentioned in Section 2, and are not
 5 based on powder feedstocks. However, because these methods are based on the
 6 deposition of heated material which bonds to previous substrate layers, the DEM
 7 methodology may be both applicable and computationally feasible. This will
 8 require the development of constitutive equations for the DEM which embody
 9 the strongly nonlinear responses of polymer materials, which may in turn require
 10 substantial revisions to the formalisms defined in Section 4. Because of the
 11 relatively low cost and widespread use of FDM in many emerging applications
 12 this effort, though involved, it is anticipated that it will offer a great deal of
 13 utility.

14 Perhaps most importantly, the completion of the short term tasks listed
 15 above will allow the simulation of loading and failure in additively manufactured
 16 test specimens. As discussed earlier, these test specimens will be of dimensions
 17 feasible for currently available additive manufacturing systems, loading frames
 18 for mechanical testing and 3D metrology systems. This will allow the func-
 19 tional validation of the DEM methodology using a data-driven mixed experi-
 20 mental/numerical technique derived from that of [89, 90]. This technique, orig-
 21 inally employed for the characterization of composite materials, will utilize an
 22 automated multiaxial test frame augmented with a full-field strain imaging sys-
 23 tem. This methodology will also be employed to calibrate the parameters of
 24 the DEM models, particularly parameters such as the dissipation term c_d of
 25 Equation (9). Geometric validation of DEM predictions will be accomplished
 26 by utilizing three-dimensional metrology systems that enable geometry recon-
 27 struction from optical or mechanical scanning of AM-built parts. Experimental
 28 validation of the DEM methodology in this fashion will allow its use for purposes
 29 such as the design, characterization, and certification of additively manufactured
 30 components.

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Sample	Scale (λ)	Shape (k)	Median (μm)
$S1$	17.3	2.60	15.0
$S2$	31.4	3.55	28.3
$S3$	41.9	2.66	36.5

Table 1: Parameters of Weibull distributions of particle diameter for the three samples measured by [84].

Description	Symbol	Value	Units
<i>Universal Properties</i>			
time step	Δt	0.025	μs
gravitation	g	$9.81 * 10^{-6}$	$\mu m/s^2$
ambient temperature	τ_e	100	$^{\circ}C$
viscous drag	c_d	0.3	–
<i>Particle Properties</i>			
density	ρ	$8.0 * 10^{-12}$	$g/\mu m^3$
normal stiffness	k_n	$1.2 * 10^3$	$N/\mu m$
friction coefficient	μ	0.25	–
thermal coefficient	k_t	$8.0 * 10^{-4}$	g/s
<i>Boundary Properties</i>			
normal stiffness	k_b	$2k_n$	$N/\mu m$
friction coefficient	μ_b	μ	–
thermal coefficient	k_{tb}	k_t	g/s
<i>Bond Properties</i>			
stiffness	k_B	k_n	$N/\mu m$
force criterion	f_{crit}	0	N
velocity criterion	v_{crit}	5	$\mu m/s$
sintering temperature	τ_s	1000	$^{\circ}C$
<i>Laser Properties</i>			
laser radius	r_e	50 – 100	μm
laser power	Q	50 – 400	W

Table 2: Listing of parameters used in the DEM simulation of SLS with 316L stainless steel.

Description	Symbol	Value	Units
model height	h	2	mm
layer height	Δh	50	μm
laser power	Q	200	W
laser radius	r_e	50	μm
laser velocity	v_l	1000	mm/s

Table 3: Slicer parameters for the first test problem.

Description	Symbol	Value	Units
model height	h	10	mm
layer height	Δh	50	μm
laser power	Q	100	W
laser radius	r_e	50	μm
laser velocity	v_l	1000	mm/s

Table 4: Slicer parameters for the second test problem.

Test	Particles	Time
Stanford Bunny	$6.02 * 10^5$	$6.5hrs$
Turbine Blade	$6.30 * 10^6$	$345hrs$

Table 5: Problem size and timing data for the two test problems.

Figure 1: Conceptual overview of powder-based additive manufacturing.

Figure 2: Overview of the Discrete Element Method. At right, the variables associated with the collision mechanics are diagrammed.

Figure 3: Visualization of the basic DEM domain Ω . Note that the scale of the particles is greatly enlarged.

Figure 4: Demonstration of the energy application methodology. Note that particle hue corresponds to the temperature field induced by the application of energy along the path defined by P .

Figure 5: Illustration of bond formation due to a concentrated heat source moving in the upwards direction. Particle hue corresponds to temperature. Bond opacity corresponds to a general notion of bond strength.

Figure 6: Illustration of the flow of execution in the C++ implementation of the DEM framework. Note the legend at upper right.

Figure 7: Numeric data and Weibull distribution parameters for three samples of 316L powder intended for use in additive manufacturing. Note the labels *S1* through *S3*, which correspond to the entries in Table 1.

Figure 8: Overview of the scraper boundary conditions for particle compaction. 1) Particles are introduced to the domain in a uniform lattice with small perturbations. 2) Particles are then allowed to settle. 3) A pair of planes travel along the x -axis, scraping away excess particles and compacting those that remain into a dense configuration. 4) The scraping planes cross the entirety of the domain; particles which exit are deleted from the simulation. 5) Laser power is applied to sinter the particles. 6) The process begins again, with the boundary conditions suitably adjusted to account for the change in overall height resulting from the buildup of layers.

Figure 9: Demonstration of the slicer input STL model (left) and one layer of the output G-code (right). Both the inner and outer perimeters are shown in black, the infill is shown in red.

Figure 10: Input STL file (left) and resulting G-code for the first DEM test simulation.

Figure 11: DEM simulation output at six points during the first layer. 1) Near the completion of the outer perimeter. 2) During the second perimeter. 3) Beginning of the infill. 4) Midpoint of the infill. 5) Infill complete, cooling begins. 6) Cooling time elapsed, immediately before introduction of particles for next layer.

Figure 12: DEM simulation output at the 4th, 23rd, and 30th layers, as well as the final output particle system. Particles which have formed no bonds are rendered in a partially transparent fashion in the first three frames, and completely transparent in the final frame.

Figure 13: Comparison of DEM input model (left) and output model (right), at the same scale and viewpoint, for the first test problem

Figure 14: Input STL file (left) and resulting G-code generated paths (right) for the second DEM test simulation.

Figure 15: DEM simulation output at four points during the one layer of the second test problem. 1) Near the completion of the outer perimeter. 2) During the second perimeter. 3) Beginning of the infill. 4) Infill complete.

Figure 16: DEM simulation output at the 50th, 100th, 170th, and 178th layers, as well as the final output particle system. Particles which have formed no bonds are not rendered, unless they are in the top layer.

Figure 17: Comparison of DEM input model (left) and output model (right), at the same scale and viewpoint, for the second test problem