Title

On Building and Investigating a New Selective Laser Melting Model Including Ray Tracing Heat Source

Abstract

A new raytracing heat source for the finite volume method(FVM) simulation of the melting process of selective laser melting(SLM) method is proposed, in order to take the complicated random packed powder bed configuration as well as the multiple optical interactions between the laser source and the material into account. The ray tracing method, namely tracking the dynamic motion and the energy exchange of individual rays is employed to simulate the Gauss distributed laser heat source, and the geometry reconstruction method based on the volume of fluid(VOF) scheme and the hexahedron structured mesh is used to dispose the complex particle arrangement generated by discrete element method(DEM). The heat source is integrated as a secondary development module of a commercial software,

A new raytracing heat source for the finite volume method(FVM) simulation of the melting process of selective laser melting(SLM) method is proposed. Compared with the conventional Gauss plane heat source or volume heat source that are common used in welding simulation, the ray tracing heat source takes the complicated random packed powder bed configuration as well as the multiple optical interactions between the laser source and the material into account, thus is more suitable for the SLM process simulation. The present study adapted the ray tracing method to the structured hexahedral mesh, thus can be

1. Introduction

Additive manufacturing, especially metal additive manufacturing is a currently burgeoning concept drawing attention from the global industry market, which aims at rapidly producing the prototype or product directly from the computer geometry files[1, 2]. Characterized by the powder bed that loads tiny metal granules layer by layer, and the laser power source that selectively melts the metal powder, selective laser melting(SLM) is among the maturest additive manufacturing technologies, earning considerable attention from the world. Compared with the conventional subtractive manufacturing methods, SLM method requires less process cycles and less raw material, and is able to manufacture many complicated structures. Despite all of these advantages, massive application of additive manufacturing is still not achieved yet, mainly because of the high costs and the unsteady quality control. Pores, denudation, cracks, poor surface roughness and balling phenomenon, these are all the common defects that may occur during the metal 3D printing process, which could do great harm to the quality and property of the final products[3-8]. In order to increase the stability and adaptability of the metal additive manufacturing, usually bunches of trail-and-error experiments need to be done to find the appropriate parameters that minimize the possibility of defect generation, which is quite time-consuming and squanders immense power, material and financial resources vastly. The popular tendency is a more widely use of numerical experiments, for which reason, a more accurate and efficient simulation system needs to be constructed.

Therefore, research on the simulations of SLM process has been enjoying a boom. Multi-scale simulations of the SLM process concentrate on different aspects of the phenomenon and mechanisms, including the melting and resolidification phenomenon, the thermal residual distortion and the metallic microstructure evolution[7, 9]. The finite element method is often employed, which is often characterized by the macro scale(). In the finite element model, continuous homogenous material with corresponding effective properties are used, as a result, the feature of the randomly packed powder and the microscopic melting behavior of the melting pool is oversimplified in these models, which is crucial to the microstructure and the final quality of the product.

Recently, the mesoscopic scale simulations have been a hot spot, where the randomly packed powder geometry is usually considered and the anisotropy of the raw material is taken into account, which brings a new demand for a suitable loading method of the heat source to the nonhomogeneous surface. Körner[10, 11] first built a 2-D Lattice Boltzmann model of the random packed powder bed, and studied about the melting, solidification and the wetting mechanisms, where the liquid-solid interface can be modelled and tracked, thus the geometry and the evolution of the melt pool is simulated. In their study, the heat source is a Gauss distributed line laser source. Besides, in the 3-D simulations, Qiu[12, 13] and Wu[14] choose to apply the Gauss distributed surface heat source, while Gu[15] uses a volume heat source.In Lawrence Livermore National Laboratory(LLNL), the ALE3D software, based on the arbitrary Lagrangian-Euler methodology, is used to simulate the three dimensional melting process[16, 17]. Their approach incorporates the multi-physics mechanisms, including the surface tension, the recoiled evaporation pressure and the dynamics of melt pool. A ray tracing heat source is used in the simulation to take the geometry of particles and the shadowing effect into account, but the multiple reflection and absorption effect is simplified and not included to save the computation. So far, the heat source model in current mesoscale SLM simulations is still not accurate and detailed enough, plane heat source and volume heat source that are widely used in welding process simulation are not able to reveal all the characteristics of the complicated interactions between the random particles and the laser source.

At the same time, there are also pioneers that make efforts to uncover the secret of laser and spheres, where some more elaborate models are used here to simulate the interactions between the laser and the packed metal powders. As early as 2002, the ray tracing method had been employed to calculate the absorptance of the laser source under the background of selective laser sintering(SLS)[18]. The model is a two dimensional model, with a consideration of the multiple reflection and heat absorption, and the heat absorptance distribution along the height direction was first induced with the help of ray tracing method. Gusarov et al. [19] then build the model of an analytical solution to the absorptance of the laser, where the powder geometry parameters are estimated and the radiation transfer equation is solved. In this model, the powder bed is considered as a thin, homogenous material, thus the uncertainty brought by the random packing of the metal particles is not taken into account. Employing the commercial software FRED, Boley et al.[20] looked into the absorptance of different metal materials, as well as investigated the influence of the powder size distribution and the laser heat source. The investigation of the heat absorptance went further in the research of Tran[21], where he analyzed and averaged the depth distribution of the heat absorptance, building a new volume heat source for the simulation of the finite element model. The use of the ray-tracing method shed substantial mesoscopic absorptance phenomenon, bring the simulation level to a new depth and precision. Yet, the investigation on the absorptance of the powder bed is individually independent to the simulation of the SLM process, and the temporal and spatial average of the calculated results leads to the elimination of the anisotropy of the heat distribution. The researches mentioned above provide the modification of the heat source parameters, however, it won’t solve the problem from fundamental.

In the present work, the ray tracing method is combined with the CFD mesoscopic simulation, in order to build a real-time varying heat source that adapts to the morphology of the powder bed. Based on the Fresnel equations, a customized subroutine that calculates the interactions between the laser and the powder bed is written, where the laser is split into numerous rays, and the interactions including the multiple reflections and the energy transfer is traced, which is close to the real condition, thus the heat distribution is provided accurately. The interface traced by VOF method is presented and reconstructed as multi facets in parallelepiped structured mesh, so the precision of the heat source matches with the meshing size. In the CFD computing program, the whole process is divided into many tiny steps. Each step, the laser heat source is moving to a new spot, and the subroutine is recalled to renew the value and distribution of the heat source, which will then be uploaded to the elements for the next step calculation, numerically, this ensures that the heat source is real time. The accuracy, precision and real-time property of the new heat source ensure that it is able to simulate the heating process, and become an important part of the meso-scale simulations of the SLM method.

2. To build the ray-tracing heat source

2.1 Reconstruction of the interface in hexahedron cells

In the simulation of melting metal powder during the SLM process, the volume of fluid(VOF) method is prevalently applied, which is a widely used numerical technique to model the free surface or fluid-fluid interface. The VOF method[22] is totally based on the idea of volume fraction, namely the volume of traced fluid inside a computational cell. When the cell is filled with the fluid, the value of fluid fraction is 1, and when the cell is empty, the value is zero. At the interface, the value is somewhere between 0 and 1. The tracking of the interface between two phases is accomplished by solving the continuity equation of the volume fraction. The properties of the materials inside the control volume are determined by the averaged value of each component’s property, for example, the density inside a cell takes a form like . In such a manner, the volume fraction and all the other thermal and dynamics properties are computed, and the interface, namely where the volume fraction satisfies , is being tracked all the time.

The Piecewise Linear Interface Calculation (PLIC) scheme is often combined with the VOF method to descript and reconstruct the sharp interface between different phases, which is the contemporary standard for most computing codes, such as Flow3D, ANSYS Fluent. In the PLIC scheme, the free surface is represented by piecewise plane segments in different cells that each has a normal vector, while the entire surface is not guaranteed to be continuous.

Subsequently, the problem arising is that how can the interaction between the laser rays and the real-time changing surface geometry be described precisely and accurately under the VOF-PLIC framework, to be more specific, that is to determine the position of a linear interface inside a cubic cell, knowing the normal vector and the volume fraction. The linear interface is often defined by , where the normal vector and the total volume fraction is known and the coefficient is to be determined. The computational zone is often a rectangular parallelepiped cell, with sides , , . And the equation is now. Without loss of generality, and is assumed. The relationship between and is not homogenous because of the differential discontinuity of the shape of the cell, thus it needs to be categorized discussed. According to the value of the fraction, several cases are induced and classified. Figure1 shows the different

Here we use to denote . The coefficient is derived purely from the geometry relationships.

(a)

(b)

In this case, should be a root of a quadric function, and the answer to this equation should be a

(c)

(d) else, if , then should satisfy the following:

(e) else, if , then a should satisfy the following relation:

In these three cases, (c)(d)(e), the equation of is a root to a cubic function.

Essentially, the problem is geometric, so there are many “if-else” blocks in the program. What’s more, there are many quadric and triple equations to solve in the program. The analytical solving method is adopted here because it can save at least half of the time compared with the numerical Newton Raphson method[23].

2.2 trilinear interpolation to eliminate the split

Now that we have determined the position of linear interfaces inside the cubic cells under the local coordinate system, the arising problem is to make sure about the continuity of the piecewise facets. In fact, the surface reconstructed by PLIC method is not continuous. Subsequently, the fake geometry of the sharp interface may lead to some drawback like the leakage of rays, the ray may leak through the split between two adjacent linear surfaces, thus the rays may go through the filled cells, and lead to an inauthentic heat distribution result. To reduce the mesh size do help to release the problem certainly, but not to solve the problem. Here a trilinear interpolation method resembling that of Ahn’s method[24] to convert PLIC surface to level set surface is used to modify the results and smooth the discontinuity.

For a better understand of the method, a 2D case is first shown for the purpose of demonstrating how the interpolation strategy works. The expression of the interface is , and position function is = , where is the coordinate of the point, and is the distance from the point to the surface. indicates that the point is at the interface, while and indicates that the point is in the exterior and interior zone respectively. For each node, there are four surrounding cells. If the cell is empty or filled, it won’t be taken into account, whilst the distance value of different cells will be averaged if the volume fraction is somewhere between 0 and 1. By this way, each node has a unique distance value, thus ensures that the entire interface is continuous.

Now that the feasibility has been discussed, the practical solution needs to be provide specifically. Considering about a parallelepiped cell, who possesses 8 vertexes distance values that determine the position of the interface. The reconstructed interface is not linear or flat any more, on the contrary, the build system is trilinear, namely the linear interpolation of 3 different directions independently. Under this scheme, although the entire surface is not differential at the intersect line between the two adjacent segments, which requires a higher order of the interpolation scheme, the modified curved surface has been able to solve the problems caused by the leaky surface. The trilinear interpolation is given by the following form:

where the is the distance from the 8 vertices to the interface inside the cell, and , , is the coordinate range of the cell. is a 3-order distance function whose highest term is , the surface is determined by .

Another important issue required to be clarified is the intersection point of a line and the trilinear surface, including the coordinate and the norm vector of the point, which is a crucial factor when calculating the reflection of the ray. After the trilinear interpolation, the surface becomes a curved surface, which means it does not have a uniform normal vector. The intersection point can be find by solving the simultaneous equation of the line and the surface, which is a one-element cubic function and the vector is calculated by differentiating the curved surface:

2.3 Traversal scheme

Another necessary issue is the propagation of the rays through the void cell, for which a classical ray traversal algorithm[25] is modified and adapted to our model.

First of all, the vectored ray should be initialized with an initial position and direction . Then the traversal of the ray through the cells should be determined step by step incrementally. For each step, the ray in a specific cell should move to its neighboring cell, either up or down or right or left or forward or back, namely the , ,, ,, directions. A major point of the traversal algorithm is to determine the accurate direction with the least computational resource. A preliminary judgement is to choose the three possible directions by the sign of the ray direction vector , for instance, if the three components of are all positive, then the ,, directions are picked out. Next step, the intersection point of the ray and the sides of the hexahedron cell are calculated respectively from the equation , where is the distance from point and. Compare the distances from the initial position to three different surfaces of the cell, and the shortest one is the real one, by which means we affirm the position of the output point, namely the initial position of next step as well.

The traversal algorithm works when the cell is empty, namely the volume fraction in the cell is zero. If the volume fraction of the cell is not zero, a judgement about whether the ray intersects with the surface inside the cell should be made.

2.4 Reflection and absorption behavior

The reflection and absorption behavior of the laser rays is one of the core mechanisms that occurs during the laser-interface interaction, which is a complex process influenced by multi parameters, such as the wave length, the absorbing material as well as the incident angle, incident polarization. To establish the model, a few assumptions are made.

First, the laser beam is consisted of a bunch of independent collinear rays, which means that each ray carries a part of the total energy and parallel to the direction of the incident laser beam. Second, the medium above the metal material is considered as the vacuum, namely, the influence of the protective gas and vapor plume is neglected, the laser energy won’t be dissipated during the propagation. Third, the laser ray hit the surface of the metal material surface, then split into a reflected wave and a refracted wave. The metal material is assumed to be opaque, that is to say, the refracted energy is all absorbed by the metal material. Last, the refracted electromagnetic wave absorbed by the metal material has all turned into heating energy, and won’t be reemitted.

Under the assumptions above, the physical mechanism of the reflection and refraction of a laser ray is characterized by Fresnel Equation:

where n is the complex refraction factor, and is the incidence angle. are the reflection ratio of s and p polarized wave respectively. When a wave is S or P polarized, it means that the electric field of the wave is perpendicular or parallel to the plane of incidence. A general incidence can be seen as the combination of S and P polarized waves. Since for natural or unpolarized electromagnetic radiation, the angle is varying all the time rapidly, the reflection ratio can be seen as a time-average of the reflection ratio of S and P polarized laser[26], that is:

When the ray reached the surface, it is supposed to reflect, and the reflection angle equals to the incidence angle. If we abstract the problem mathematically, given the vector of the ray and the norm vector of the surface, which is shown in the above chapter, the direction vector of the reflected ray is straight-forward using Householder transformation:

where is the identity matrix, is the incident vector, and is the reflection matrix. The reflected vector should be .

2.5 Algorithm of the ray-tracing program

In the mesoscopic simulation of the SLM process, the heat transfer is governed by the energy conservation equation:

,

where is the heat transfer coefficient, and is the specific heat capacity, and is the heat source term. Our job is to determine the source term, namely the heat energy absorbed by per mass of the metal material.

In this part, we put forward a total solution to combining the ray tracing heat source with the CFD simulation model. The heat source part can be complied as a macro or subroutine, which will run independently and exchange data with the main CFD program during each calculating time step.

First the powder bed configuration is generated using DEM method, which is transferred to geometry file that supported by the CFD software, usually STL, for the purpose of building the CFD model. Then the important data of the targeted heated region, including the mesh information, the volume fraction and surface normal vector in the cells, is extracted, to which the ray tracing subroutine is accessed to.

Next, the ray-tracing program is exploited to calculate the heat source distribution of the random packed powder bed. First the laser is separated into many independent rays, each carries a part of energy determined by the relevant position of the ray, usually the distribution of the laser source is Gauss distribution. After that the VOF geometry is reconstructed to find the exact position of the interfaces under referred hexahedron cell reconstruction algorithm. First the analytical expressions of the interfaces are found, then trilinear interpolation is exerted to smooth the split between different interfaces. After the reconstruction of the geometry of target zone, simulation of the trace of each ray is carried out. The traversal of the rays is traced cell by cell, based on the traversal algorithm. if the ray reached a cell that possesses a no-zero volume fraction, the intersection point of the ray and the interface shall be calculated. The reflection model is called and executed when the intersection point is inside the cell, which calculates the incident angle and changes the direction of the ray, and does the exchange of energy between the ray and the cell. Otherwise, the ray will keep on its propagation. The tracing of a ray keeps working until one of the listed circumstance occurs: 1. The ray leaks out of the target zone, from the top surface or the side surfaces. 2. After multiple reflections, the energy of the ray is lower below 0.1% of the initial value. 3. In case the endless loop caused by any unexpected bug, the loop is forced to stop when reaching a max number of traversal.

Finally, after a whole loop, the cells’ energy exchange history along with the ray propagation history is stored in an array, which can be returned as the element distributed heat source by the external numerical software directly or be written into files for the further analyzation.

3. results and analyze

3.1 discussion on the mesh size and the ray numbers

As a heat source integrated in the CFD program, the ray tracing program is characteristiced by the structured hexahedron mesh, which makes the calculating result sensitive to the mesh size. The determination of the mesh size is an important issue in SLM simulations. A coarse meshing may induce the lack of precision, while too fine a meshing could occupy too much computing resource, for which reason, in this study, a series of simulations with different mesh precisions are carried out to shed light on the influence of mesh size.

A powder bed with a mean radius size of 13 microns, is generated in the DEM model, and then meshed in different sizes of 0.5μm,1μm,2μm and 4μm. Then the heat distribution, especially accumulated heat distribution along the height direction, is analyzed and compared to check the impact of different mesh sizes. From the figure, the heat absorptance distribution results drawn from different mesh-size simulations share the similar trend and value. The absorptances of the substrate in different cases are also identical.

For the quantified analyzation, a dimensionless number is introduced, where is the ratio of the mesh size and is the characteristic length of the geometry. Using the mean radius as the characteristic length, the coefficient of determination under different is analyzed. The results indicate that the heat source results are very close when is smaller than 0.15, which can be an important criteria to select the mesh size.

Besides the mesh size, the ray numbers are also a crucial factor that effect the final result of the heat distribution. The very first step of the ray-tracing simulation of the laser heat source is to split the laser heat source into many separated rays, the total number of which may produce an effect on the final result. Instead of the randomly generated rays, the rays in our model is uniformly arranged to save the computing resources this step. If the density of the rays is low, the rays may not enough to reveal the distributional feature of the laser source. Since the ray interacts with the geometric surface of the powder bed, and the powder bed is meshed and reconstructed as contiguous surfaces in different cell, naturally, a new parameter n should be introduced to represent the density of the rays, which means the number of the rays that perpendicularly go through a particular rectangular parallelepiped cell.

Reference

[1] Wong K V, Hernandez A. A review of additive manufacturing [J]. ISRN Mechanical Engineering, 2012, 2012(10.

[2] Wohlers T. Wohlers report 2018 [M]. Wohlers Associates, Inc, 2018.

[3] Kruth J-P, Levy G, Klocke F, et al. Consolidation phenomena in laser and powder-bed based layered manufacturing [J]. CIRP annals, 2007, 56(2): 730-59.

[4] Leuders S, Thöne M, Riemer A, et al. On the mechanical behaviour of titanium alloy TiAl6V4 manufactured by selective laser melting: Fatigue resistance and crack growth performance [J]. International Journal of Fatigue, 2013, 48(300-7.

[5] King W E, Barth H D, Castillo V M, et al. Observation of keyhole-mode laser melting in laser powder-bed fusion additive manufacturing [J]. Journal of Materials Processing Technology, 2014, 214(12): 2915-25.

[6] Debroy T, Wei H, Zuback J, et al. Additive manufacturing of metallic components–process, structure and properties [J]. Progress in Materials Science, 2017,

[7] Sames W J, List F, Pannala S, et al. The metallurgy and processing science of metal additive manufacturing [J]. International Materials Reviews, 2016, 61(5): 315-60.

[8] Zhou X, Liu X, Zhang D, et al. Balling phenomena in selective laser melted tungsten [J]. Journal of Materials Processing Technology, 2015, 222(33-42.

[9] Francois M M, Sun A, King W E, et al. Modeling of additive manufacturing processes for metals: Challenges and opportunities [J]. Current Opinion in Solid State and Materials Science, 2017, 21(LA-UR-16-24513):

[10] Körner C, Bauereiß A, Attar E. Fundamental consolidation mechanisms during selective beam melting of powders [J]. Modelling and Simulation in Materials Science and Engineering, 2013, 21(8): 085011.

[11] Körner C, Attar E, Heinl P. Mesoscopic simulation of selective beam melting processes [J]. Journal of Materials Processing Technology, 2011, 211(6): 978-87.

[12] Qiu C, Panwisawas C, Ward M, et al. On the role of melt flow into the surface structure and porosity development during selective laser melting [J]. Acta Materialia, 2015, 96(72-9.

[13] Panwisawas C, Qiu C, Sovani Y, et al. On the role of thermal fluid dynamics into the evolution of porosity during selective laser melting [J]. Scripta Materialia, 2015, 105(14-7.

[14] Wu Y-C, San C-H, Chang C-H, et al. Numerical modeling of melt-pool behavior in selective laser melting with random powder distribution and experimental validation [J]. Journal of Materials Processing Technology, 2018, 254(72-8.

[15] Gu D, Ma C, Xia M, et al. A Multiscale Understanding of the Thermodynamic and Kinetic Mechanisms of Laser Additive Manufacturing [J]. Engineering, 2017, 3(5): 675-84.

[16] Khairallah S A, Anderson A T, Rubenchik A, et al. Laser powder-bed fusion additive manufacturing: Physics of complex melt flow and formation mechanisms of pores, spatter, and denudation zones [J]. Acta Materialia, 2016, 108(36-45.

[17] Khairallah S A, Anderson A. Mesoscopic simulation model of selective laser melting of stainless steel powder [J]. Journal of Materials Processing Technology, 2014, 214(11): 2627-36.

[18] Wang X, Laoui T, Bonse J, et al. Direct selective laser sintering of hard metal powders: experimental study and simulation [J]. The International Journal of Advanced Manufacturing Technology, 2002, 19(5): 351-7.

[19] Gusarov A, Kruth J-P. Modelling of radiation transfer in metallic powders at laser treatment [J]. International Journal of Heat and Mass Transfer, 2005, 48(16): 3423-34.

[20] Boley C D, Khairallah S A, Rubenchik A M. Calculation of laser absorption by metal powders in additive manufacturing [J]. Appl Opt, 2015, 54(9): 2477-82.

[21] Tran H-C, Lo Y-L. Heat transfer simulations of selective laser melting process based on volumetric heat source with powder size consideration [J]. Journal of Materials Processing Technology, 2018, 255(411-25.

[22] Hirt C W, Nichols B D. Volume of fluid (VOF) method for the dynamics of free boundaries [J]. Journal of computational physics, 1981, 39(1): 201-25.

[23] Scardovelli R, Zaleski S. Analytical relations connecting linear interfaces and volume fractions in rectangular grids [J]. Journal of Computational Physics, 2000, 164(1): 228-37.

[24] Ahn J, Na S-J. Three-dimensional thermal simulation of nanosecond laser ablation for semitransparent material [J]. Applied Surface Science, 2013, 283(115-27.

[25] Amanatides J, Woo A. A fast voxel traversal algorithm for ray tracing; proceedings of the Eurographics, F, 1987 [C].

[26] Zohdi T I. Rapid simulation of laser processing of discrete particulate materials [J]. Archives of Computational Methods in Engineering, 2013, 20(4): 309-25.