Smoothed Particle Hydrodynamics Modeling of the Multi-layer Laser Powder Bed Fusion Process

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Abstract

The need for materials and process optimization in laser powder bed fusion (LPBF) goes hand in hand with its numerical simulation capabilities. This work lays the groundwork for developing an efficient predictive tool that can ultimately capture manufacturing defects in 3D multi-layer LPBF simulations and generate insights into possible ways to avoid or mitigate them. As a first step towards that end, we present a 2D numerical framework based on the smoothed particle hydrodynamics (SPH) method featuring a new powder application. SPH simulations with the successive building of ten layers using two different laser powers are performed to show how the unevenness of layers develops during LPBF and how it can be alleviated, e.g., by adjusting the laser power.

Keywords: Additive manufacturing; Laser powder bed fusion; Multi-layer; Simulation; Smoothed particle hydrodynamics

1. Introduction

Laser powder bed fusion (LPBF) is the most prevalent additive manufacturing (AM) technique for fabricating metal parts with complex shapes. An overview of recent industrial and technological advances in AM of metals can be found in [1]. In LPBF, as illustrated in Figure 1, a moving laser spot is utilized to selectively fuse thin layers of powder material through a predesigned scan pattern. The rapid industrial take-up of this technology in the past few years has made it indispensable to establish an in-depth understanding of the physics of the process for its broader applications. Numerical simulation of LPBF can help achieve this goal by generating valuable insights into the process, which are notoriously difficult or impossible to obtain solely from the experiment.

For a complete representation of the multi-layer LPBF process, the numerical simulation framework needs to repeatedly generate the powder layer and discretize the thermo-fluid dynamics equations. On the one hand, this iterative procedure is computationally very expensive as the number of computational elements increases layer by layer, and the runtime does not scale linearly. On the other hand, several complications due to coupling issues exist as the methods used in the literature for the powder application and melting simulation are usually not the same. For instance, Cao and Guan [2] presented a 3D multi-layer single-track LPBF simulation framework using the discrete element method (DEM) for modeling the powder bed and the finite volume method (FVM) for the fluid flow. They utilized a multi-threading scheme to speed up the simulation; however, the calculation time reported for building eight layers of LPBF is still within 5-12 days for different layer thicknesses and depending on the number of elements. Another effort into a multi-layer simulation is the work of Rausch et al. [3] using a 2D mesoscopic approach based on the lattice Boltzmann method (LBM). Each new layer in this framework was coated by employing a rainfall-like deposition scheme to simulate the buildup of 100 layers. Some crucial phenomena such as the recoil pressure and Marangoni effects are missing from the physical model of [3]. Moreover, a three-dimensional extension of this numerical framework is necessary for more accurate and reliable investigations.

As an alternative to the mesh-based and CFD approaches, the class of mesh-free particle methods has also been utilized for modeling LPBF processes on the powder scale. Smoothed particle hydrodynamics (SPH) is currently the most established...
mesh-free method for additive manufacturing simulations and is the main focus of this paper. Besides its unique strength in handling large deformations and violent free-surface flows, SPH offers another feature, which is particularly attractive for multi-layer LPBF simulations. The SPH method can be used for the powder bed deposition, meaning no coupling to other numerical methods (e.g., DEM) is needed. Recent 2D SPH simulations of LPBF include the high-fidelity modeling approach of Russell et al. [4], and the multi-resolution scheme of Afrasiabi et al. [5]. Thanks to the runtime acceleration by parallel computing, the SPH codes have made significant progress in presenting 3D results. The GPU-based single-track LPBF simulations of Weirather et al. [6] and Fürstenau et al. [7] are two published works worth mentioning. Most recently, Wimmer et al. [8] demonstrated the capability of SPH for the simulation of in-situ alloying in LPBF. All these publications reveal the great potential of SPH for further developments in modeling LPBF. Nevertheless, the simulation domain of all these papers is limited to only one powder layer.

In this work, we take the first steps towards the development of an efficient 3D SPH code for modeling multi-layer LPBF processes. The 2D numerical framework presented here covers a layer-by-layer powder deposition model while accounting for all dominant physical phenomena, including surface tension forces and Marangoni effects. The method captures the temperature distributions, material phase, melt pool dimensions, and solidified track geometries within a reasonable amount of calculation time, generating valuable insights into how the unevenness of layers develops during the process. The computer code used for producing the numerical results relies on our previous developments for CFD [9, 10], thermal [11, 12, 13], and thermomechanical manufacturing [14, 15] applications.

2. Materials and Methods

This section explains the computational framework of the present study in brief. For a more detailed description of the methodology and its theoretical background, please refer to our previous work in [5]. For modeling a multi-layer LPBF process, it is necessary to include the powder deposition step in the layer-by-layer melt pool simulation. Consequently, a complete numerical modeling framework for LPBF would consist of two modules:

1. Thermo-fluid dynamics module
2. Powder layer generation module

These two modules are considered independent and executed separately, meaning the thermo-fluid dynamics module is inactive while the powder layer generation is running and vice versa.

2.1. Thermo-fluid dynamics module

The fluid motion in LPBF can be determined by solving the Navier–Stokes equations, assuming the flow of the molten material is incompressible. These equations ensure the mass, momentum, and energy conservation of the system via

\[
\dot{\rho} = -\rho \nabla \cdot \vec{v}
\]

(1)

\[
\rho \vec{v} = -\nabla p + \mu \nabla^2 \vec{v} + \rho g + \vec{b}
\]

(2)

\[
\rho c_p T = \frac{\varepsilon}{\tau} : \nabla \vec{v} + \nabla \cdot (k \nabla T) + Q_l
\]

(3)

where \( \rho \) is the density, \( \vec{v} \) the velocity, \( p \) the pressure, \( g \) the unity tensor, \( \mu \) the viscosity, \( \rho g \) the gravitational acceleration, \( \vec{b} \) volumetric body forces, \( c_p \) the specific heat capacity, \( T \) the temperature, \( \tau \) the shear stress tensor, and \( k \) the thermal conductivity. The term \( Q_l \) in Equation (3) represents the input energy of the system provided by the laser beam, which is modeled here as a volumetric heat source based on the Beer-Lambert law. The intensity of the laser in the radial direction is computed from a normalized Gaussian distribution as

\[
I(r) = \frac{2P_l}{\pi R^2} \exp\left(-\frac{2r^2}{R^2}\right)
\]

(4)

if \( P_l \) is the laser power and \( R \) the laser beam radius. In order to enforce the incompressibility condition, a commonly-used equation of state as

\[
p = c_0^2 (\rho - \rho_0)
\]

(5)

is additionally considered, in which \( c_0 \) denotes the (artificial) speed of sound. Surface tension forces, thermo-capillary and recoil pressure effects are also taken into account. Details about the mathematical formulations of these terms and how they are implemented into an SPH framework have been already given in [6, 5], and are not revisited here.

As shown by previous studies such as [16] and [17], the spatially discretized form of the Navier-Stokes equations (i.e., Equations (1)-(3)) in a Lagrangian frame using the SPH method can be written as
\[
\langle \rho_i \rangle \approx \rho_i \sum_j \left( \frac{\delta_{ij} + 2\delta h c_0 \frac{\hat{p}_{ij}}{|\vec{r}_{ij} - \vec{r}_j|^2}}{\eta^2} \right) \cdot \nabla W_{ij} \quad V_j
\]  
\[
\langle \psi_i \rangle \approx \sum_j \frac{1}{\rho_i} \left( \frac{\hat{p}_{ij}}{\Gamma_j} \right) \nabla W_{ij} V_j + \frac{1}{\rho_i} \left( \frac{2\mu_{ij}}{\mu_i + \mu_j} \right) \pi_{ij} \nabla W_{ij} V_j + \frac{s + 1}{\rho_i} b
\]  
\[
\langle T_i \rangle \approx \sum_j \frac{1}{c_p \rho_i} \left( \frac{\mu_{ij}}{\mu_i + \mu_j} \right) \frac{m_i}{\rho_i} \pi_{ij} \psi_{ij} \cdot \nabla W_{ij} + \frac{1}{c_p \rho_i} \left( \frac{4k \kappa_j}{k_i + k_j} \right) \frac{m_i}{\rho_i} T_{ij} \left( \frac{\ell_{ij}}{|r_{ij} - \vec{r}_j|^2 + \eta^2} \right) \cdot \nabla W_{ij}
\]

where \( \bullet = \bullet_i - \bullet_j \) for abbreviation, \( V_j = m_j/\rho_j \) is the SPH integration volume, \( \pi_{ij} = 2(n_D + 2)(\delta_{ij} - |\vec{r}_{ij} - \vec{r}_j|^2) / n_D^2 \) with \( n_D = 2 \) for a 2D problem, \( \Gamma_j = \sum_i V_j W_{ij} \) is a renormalization coefficient used in SPH free surface problems, and \( \eta = 0.0001 \) a smoothing parameter for the \( \delta \)-SPH scheme of Antuono et al. [17]. Throughout this work, the SPH kernel \( W \) is a Wendland quintic function [18] with the smoothing length \( h \). In Equation (8), the multi-phase SPH scheme of Cleary [19] is used for discretizing the Laplace operator. Also, a small parameter \( \eta = 0.1h \) is inserted in the denominator to prevent the fraction from singularity.

2.2. Powder layer generation module

A method for deposition of metal powder is required for the layer-wise build-up of the solidified melt track. Within the computational framework of this paper, the powder layer generation is modeled by taking a rainfall approach into account. In this procedure, powder grains are generated above the substrate and fall on the previous (solidified) track following their gravitational body force. Each single powder grain consists of several SPH particles depending on the spatial resolution of the simulation. To reduce the computational effort, we carry out the rigid body simulation within an exterior simulation block where the thermo-hydro dynamics module is disabled. Conversely, no rigid body motion is considered during the laser scanning simulation.

Our rigid body motion implementation follows the method presented by Rubens et al. [20] based on a penalty-based spring dash-pot model. For simplicity, the interaction is limited to the normal force contribution only, i.e., no tangential frictional force is considered. A graphical representation of this model for two contacting powder particles is shown in Figure 2. In essence, the approach is similar to the discrete element method (DEM) formulation with a slight difference of calculating the collision forces along the local normal direction at the point of contact. It assumes each powder particle to be a rigid body \( k \) and applies the following laws of motion

\[
\dot{\psi}_k = \frac{f_{\text{ext}}}{m_k} \quad \dot{\omega}_k = \frac{M_{\text{ext}}}{I_k}
\]  

where \( \psi_k \) is the total velocity, \( f_{\text{ext}} \) the external force, \( m_k \) the mass, \( \omega_k \) the angular velocity of rigid body \( k \), \( M_{\text{ext}} \) the external torque, and \( I_k \) the second moment of inertia with respect to the center of mass \( M \) of \( k \). The collision force between particles \( i \) and \( j \) is computed from the non-linear Hertzian elastic contact model. This term is denoted by \( f_{\text{col}} \), which includes the repulsive and damping components as

\[
f_{\text{col}} = k_i \delta_{ij}^{3/2} n_s - c_i \delta_{ij}^{1/4} \delta_{ij} n_s
\]

in which \( \delta_{ij} \) and \( \delta_{ij} \) are referred to as a positive particle overlap and the rate of penetration, respectively, which are calculated from

\[
\delta_{ij} = \Delta x - |\vec{r}_{ij}|
\]

\[
\dot{\delta}_{ij} = (u_i - u_j) \cdot n_s
\]

where \( \Delta x \) denotes the uniform particle spacing, \( |\vec{r}_{ij}| \) the distance between particles, and \( n_s \) the normal vector for each powder particle. The spring constant \( k_i \) and damper coefficient \( c_i \) are defined by

\[
k_i = 4 \frac{3}{2} E_i \sqrt{\frac{\Delta x}{2}}
\]

\[
c_i = C \sqrt{6 m_i E_i \sqrt{\frac{\Delta x}{2}}}
\]

where the averaged mass and Young’s modulus are defined, respectively, as

\[
m_{ij} = \frac{m_i m_j}{m_i + m_j} \quad E_{ij} = \frac{E_i E_j}{E_i(1 - \nu_j) + E_j(1 - \nu_i)}
\]
with \( \nu \) denoting the Poisson ratio and \( C_n \) the ratio of the collision. Finally, the resultant force and torque of each powder particle \( k \) is calculated by adding the respective contributions of its SPH particles via

\[
\begin{align*}
\mathbf{f}^\text{ext}_k &= \sum_{i \neq k} \mathbf{f}^\text{col} \sum_{i \neq k} \sum_{j \neq k} \mathbf{f}^\text{col}
\mathbf{M}^\text{ext}_k &= \sum_{i \neq k} \mathbf{M}^\text{col} \times \mathbf{f}^\text{col} \times \mathbf{f}^\text{col} \times \mathbf{f}^\text{col}
\end{align*}
\]

where \( \mathbf{f}^\text{col} \) is the distance vector to the center of mass. Equation (17) can now be solved for the powder particles in order to model the deposition step. Once the powder particles are settled down, no further solid displacement is permitted and the laser starts scanning the powder layer.

In the present rainfall approach, the solidified track and previously deposited grains serve as fixed boundary particles for the next layer. Additionally, wall boundaries are temporarily created at the two edges of each laser track to prevent metal grains from falling off the substrate. The powder layer generation module is run over a time interval of 1 s, providing enough time for the powder particles to settle down. If a powder layer contains more than one row of grains, the code takes a user-defined threshold and deletes the powder grains exceeding the desired layer thickness. This trimming procedure facilitates a flat powder bed surface, which mimics the recoating process in some ways. The whole procedure is repeated after each layer is fully scanned and completely solidified. More details regarding the layer thickness and cooling time between the layers are given in the results section.

### 3. Results and Discussion

We present the results of two multi-layer LPBF simulations using a 100 and 150 W laser at a constant scan speed of \( v_\text{s} = 0.8 \) m/s. These models allow for the successive building of 10 powder layers to investigate the prediction capability of our SPH solver for capturing possible defects in LPBF. The substrate and metal powder material used here were 316L stainless steel, with the properties summarized in Table 1. Please note that we use a 100x higher viscosity for “solid” phase particles to simulate the mushy region, with a linear interpolation based on the liquid weight fraction (see \( \mu \) in Table 1). The “liquid” dynamic viscosity is 0.01 Pa s, similar to the approach used by [4, 5]. Also, the absorption coefficient \( \alpha \) is constant, and the temperature dependence of absorptivity is not considered in our model. The diameter of powder grains was \( d = 40 \pm 5 \) \( \mu \)m. The layer thickness is set to 50 \( \mu \)m. The Gaussian laser beam with a radius of 27 \( \mu \)m scans the odd layers (1,3,5, ...) from left to right and the even layers (2,4,6, ...) from right to left. That is, the Gaussian-shaped beam starts printing the part from left to right and moves in a snake-like path among layers. Ten layers were built and simulated using this strategy.

The computational domain has a constant length of 1.2 mm and a variable height that dynamically increases after scanning each layer. At the initial configuration, the regular particle spacing is 8 \( \mu \)m and one powder layer containing 25 to 30 uniformly-spaced grains is deposited on a fixed 1.2x0.12 mm solid substrate. For layers 2 to 10, the powder deposition procedure in the simulation follows a rainfall approach and starts after each scanned track is fully solidified. To impose this condition, an extra cooling time of 3 (\( t_c/v_\text{s} \)) is added to the scan time of each track, where \( t_c \) is the track length and \( v_\text{s} \) the scan speed. The thermal boundary conditions of this problem include heat exchange with the environment via radiation and convection through all open surfaces and a constant temperature of \( T_0 = 293 \) K on the bottom of the substrate (i.e., heat sink).

Table 3 shows the temperature distribution and the computed shapes of the melt pool at the first layer for different laser powers. These four screenshots are taken after scanning 0.7 mm of the track, which is sufficient for the melt pool size to reach a quasi-steady state. Table 2 summarizes the results of our first layer simulation alongside the data provided by [21]. In order to visualize the melt pool and calculate its dimensions, we interpolated the molten flow interface by extracting the SPH particles whose fraction of fluid was equal to 1 (i.e., the red particles in Figure 3). With this strategy, melt pool characteristics such as its length, depth, surface area, and average/maximum temperature can be calculated and analyzed. Through a first observation, one can see that the melt pool dimensions for the case of using a 150 W laser are significantly higher than a 100 W laser, which is unsurprising. Increasing the laser power by 50%, from 100 to 150 W, led to a 107% increase in the melt pool length, from 0.288 to 0.582 mm. Recent studies such as the experimental investigation of Guo et al. [22] have already confirmed this effect, pointing out that: Among different process parameters, laser power has the highest impact on the melt pool geometry.

<table>
<thead>
<tr>
<th>Property</th>
<th>Symbol</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ambient temperature</td>
<td>( T_0 )</td>
<td>293</td>
<td>K</td>
</tr>
<tr>
<td>Melting temperature</td>
<td>( T_m )</td>
<td>1723</td>
<td>K</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>( k )</td>
<td>20.93</td>
<td>W/(m K)</td>
</tr>
<tr>
<td>Convection coefficient</td>
<td>( h_c )</td>
<td>20</td>
<td>W/(m² K)</td>
</tr>
<tr>
<td>Specific heat capacity</td>
<td>( c_p )</td>
<td>711.2</td>
<td>J/(kg K)</td>
</tr>
<tr>
<td>Dynamic viscosity</td>
<td>( \mu )</td>
<td>1</td>
<td>Pa s</td>
</tr>
<tr>
<td>Density</td>
<td>( \rho )</td>
<td>7332</td>
<td>Kg/m³</td>
</tr>
<tr>
<td>Absorption coefficient</td>
<td>( \alpha )</td>
<td>0.27</td>
<td>–</td>
</tr>
<tr>
<td>Emissivity coefficient</td>
<td>( \epsilon )</td>
<td>0.40</td>
<td>–</td>
</tr>
</tbody>
</table>

Table 2. Comparison of the melt pool dimensions with the data from [21].

<table>
<thead>
<tr>
<th>Track energy (J/m)</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Ref. [21]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melt pool length (mm)</td>
<td>0.288</td>
<td>0.582</td>
<td>0.275</td>
</tr>
<tr>
<td>Melt pool depth (mm)</td>
<td>0.049</td>
<td>0.078</td>
<td>0.045</td>
</tr>
</tbody>
</table>
While the regularity of the melt pool changes more noticeably with the increasing number of layers, the overall shape of the melt pool stays more or less the same among layers. Shown in Figure 4 are the melt pools for different laser powers, shortly after the beam has scanned the last layer. As mentioned before, the highlighted green areas in this figure that represent the melt pool are determined by isolating the SPH particles with a fluid fraction of 1. It can be seen that the melt pool in both cases exhibits a teardrop shape due to the rapid scan speed of the LPBF process. See [23] for more explanation. At this time step, the beam has already scanned the tenth layer and is inactive in the simulation. Therefore, the melt pool is no longer at a steady state, and its dimensions are not comparable to those presented in Figure 3.

To further investigate the impact of laser power on the unevenness developing among layers, it is helpful to compare the layer-by-layer building process for different heat inputs. Figure 5 displays the temperature evolution of the LPBF simulations at four different layers for a 100 and 150 W laser power with the same scan speed. Quite clearly, the maximum and average temperatures of the 150 W case are higher than the other. The laser beam travels in the direction of negative x-axis as the number of chosen layers is even in all cases. For the two LPBF simulations performed, there was no remarkable difference between the surface quality of the 100 W and 150 W cases at the first layer (see Figure 3). Nevertheless, irregular melt pool shapes were formed at higher layers as a result of generating an uneven powder layer. Given the processing condition, excessive surface roughness can be observed at the third and fifth layers using a 100 W laser, as shown in Figure 5. This unevenness stems from a relatively more wobbly surface of the previous (solidified) track, which, in turn, indicates improper fusion-based bonding among layers.

Through graphical construction, Figure 6 compares the identified porosity locations and the surface quality of the final part for different laser powers. The void areas are recognized as porosity if they encompass at least a stencil of four SPH particles. This criterion is proposed to distinguish between the physics-induced porosity and numerical resolution artifacts. The comparison shows that the probability of obtaining an uneven surface with a 100 W laser in this setup is higher. The voids observed here for the case of 100 W are eliminated by increasing the laser power to 150 W, as shown in Figure 6-(b). Regardless of the ad hoc void detection criterion defined here, a high-resolution simulation would be required to verify whether or not the voids in Figure 6-(a) are present at a smaller discretization size.

Furthermore, the final surface of the part printed by a 150 W looks flatter than the one produced by a 100 W laser. This effect can be related to an uneven powder bed surface caused by insufficient fusion from previous layers that would eventually lead to higher surface roughness. A (visual) comparison of the red and blue dashed lines in Figure 6 supports the provided argument.
4. Conclusion

We developed a new simulation tool and demonstrated its capability for predicting manufacturing flaws in laser powder bed fusion (LPBF) processes. The computational framework of this study adopts the smoothed particle hydrodynamics (SPH) method for modeling the complex thermo-hydro dynamic phenomena in LPBF but also relies upon the efficiency and robustness of this choice to present the first multi-layer LPBF simulation using SPH. A summary of the key points concluded from this investigation is as follow:

- The short computation cycles due to the 2D simplification and efficient powder generation module allowed for modeling multiple layers of the building process. Calculation times are manageable, i.e., a full 10-layer simulation can be terminated in a few hours using a single CPU core.
- Unevenness of layers resulting from irregular melt pool shapes was qualitatively captured by the SPH method in a multi-layer LPBF simulation.

Although we provided a rough comparison of the simulated melt pool dimensions with some available experimental data from the literature, it is still necessary to conduct original LPBF experiments to fully validate the code and evaluate its performance for multi-layer printing processes. This would be an immediate continuation of the present study. Another follow-up work focuses on the runtime reduction by parallel computing to enable a three-dimensional simulation. Further developments can also go in the direction of improving the powder bed model and providing a consistent set of material parameters.

References


