Steady state numerical calculation of the melt-pool shape

E V Avdeev

1Samara National Research University, Moskovskoe Shosse 34A, Samara, Russia, 443086

e-mail: j-avdeev@yandex.ru

Abstract. A two-dimensional steady-state melting problem is numerically simulated. This task arose during the Selective laser melting (SLM) additive process technology modeling project. The initial problem is the formation of residual stresses and, as a consequence, the appearance of accumulated deformations (inherent strains) and distortion of final production shape. As the solution of this initial problem suggested the development of its own appropriate software tool. The development process was divided into 5 stages. Stage 1 is to model the geometric size of the molten bath. A comparison of the results obtained within OpenFOAM (laserConvBC) and results from a similar article.

1. Introduction
Selective laser melting (SLM), also known as direct metal laser sintering (DMLS) or laser powder bed fusion (LPBF), is a rapid prototyping, 3D printing, or additive manufacturing (AM) technique designed to use a high power-density laser to melt and fuse metallic powders. In SLM, the three-dimensional model of the manufactured part is divided into layers with a thickness from 20 to 100 microns. In each layer, a local heat source (laser beam, etc.) melts metal powder particles and forms "tracks" (welded tracks, welds) which are located at a certain distance from each other. The process of manufacturing parts of SLM includes the heating, melting and solidification of the material by a moving heat source, such as a laser, layer by layer. As a result, different parts of the production component get different reheat and cool cycles. Spatially modified thermal cycles lead to the formation of residual stresses and, as a consequence, to the appearance of accumulated deformations (inherent strains) and distortion of final production shape.

2. General problem statement
The general problem is software tool development that implements a multiscale approach based on the finite element method, which provides a faster determination of residual stresses and distortions for SLM production components. Residual stresses and distortion determination approach includes the calibration of the heat source, the analysis of scanning strategies (shading), the generation of the so-called "mechanical layer equivalent" and its integration into the accelerated structural analysis.

A similar approach was recently implemented in commercial software such as Simufact Additive by MSC Software. As the practice of using the Simufact Additive has shown, the simulation results are in very good agreement with experimental measurements. The usage of commercial software with closed source code brings the following limitations: closed source code, complexity/impossibility of detailed model correction.
3. General problem solution stages

Stages of the proposed software development are following:

- **Stage 1.** Solving the problem of temperature distribution in the molten bath in a stationary setting. Depending on the shape and curve of the energy distribution of the laser beam, the melt bath geometry is modeled by solving the heat equation with the substrate/melted layer boundary conditions, unmelted powder, inert gas environment and based on the finite volume method. The solution is the stationary state equation and should give a three-dimensional description of the melting isotherm.

- **Stage 2.** Solving the temperature distribution problem in the alloyed layer in a quasi-dynamic formulation depending on the technological parameters (speed and beam scanning step), descriptions of the geometry of the moving melt bath and the temperature in the melt bath found in the first stage. This allows us to describe the front of the transition from almost zero conductivity (outside the conduction front) to conductivity immediately ahead of the melt front and to determine the boundaries of the "equivalent mechanical layer" for the next stage.

- **Stage 3.** Solving coupled thermal problems and structural analysis problems in the top row of finite elements of an “equivalent mechanical layer” containing a fused layer of material. Determination of accumulated deformations in the "equivalent mechanical layer".

- **Stage 4.** Solving the problem of structural analysis for finite volumes of other lower layers. Calculate accumulated deformations load from the “equivalent mechanical layer”. Calculate the elastic response from the applied load.

- **Stage 5.** As a result of the solution, the thermal displacements of the finite volume model are determined. Inverting these offsets applied already to the nodes of the STL-file of the geometric model of the production component, i.e. Pre-adjusting the model for negative values of these displacements before generating the control program for building a part, it is possible to level the effects of thermal stresses.

This paper describes the results of Stage 1. In this stage, I simulated the temperature distribution and the melt pool borders, during particles melting with a laser beam.

4. Temperature distribution in the molten bath. Problem description

This paper presents the results of a simulation of the temperature distribution with OpenFOAM library and a comparison of the obtained results with similar works [1, 2], that used commercial tools COMSOL, Ansys and shows proper agreement with experimental results. Several existing studies [3, 4, 5, 6] have employed a basic heat-transfer model to investigate the thermal behavior in SLM of metal powders such as stainless steel and titanium alloys and have proposed techniques to simulate the addition of layers with time.

OpenFOAM library was chosen as the most advanced opensource tool, which has set primitive or almost developed features for simulating heating, melting, adding material and calculating the resulting thermal stresses. The first release of the OpenFOAM library was released in 2004 and currently, there is a fairly large community of users, specialists, and enthusiasts who are developing various tools based on the OpenFOAM tools. One example of such developments was a module laserConvBC that implements the boundary condition for the transfer of thermal energy by a laser, developed by Tobias Holzmann [7]. This module was used in the current work.

OpenFOAM module laserConvBC offers features like:

- Reducing the laser power based on some user functions.
- Using temperature-dependent thermal conductivity field.
- Heating and quenching.
- Two different motion modes: linear point-to-point and circular.
- Arbitrary laser sources.

For simplicity, a small plate (1E-6 x 1E-6 x 5E-8 m) was chosen as the geometry describing the powder layer. figure 1 shows the 3D geometry of the powder layer.
The following assumptions are made in this simulation:

- The composite powder bed was assumed to be homogeneous and continuous.
- The heat flux from the laser beam was modeled as Gaussian-distributed heat flux and was given directly on the top of the composite powder bed.
- The simulation did not take into account heat loss at the phase transition.
- The laser spot was assumed to have a circular shape.
- The convective heat transfer coefficient between the environment and the powder bed was assumed to be a constant and independent of temperature.

5. Boundary conditions

Boundary conditions are chosen according to the work of Peyre [1] to make a comparison. Boundary conditions are shown in Table 1.

| Value name                        | Designation     | Value |
|-----------------------------------|-----------------|-------|
| Initial temperature, [K]          | \( T_0 \)       | 300   |
| Heat Transfer Coefficient for heating, [W/m²*K] | HTCheating | 150   |
| Scanning speed, [mm/s]            | heatingTime     | 1000  |
| Laser power, [W]                  | power           | 350   |
| Spot size X, [m]                  | sigmaX          | 7E-8  |
| Constant heat conduction, [W/(m*K)] | kValue         | 10    |
| Material thermal diffusivity (Aluminium powder), [m²/s] | DT             | 5E-06 |

6. Mesh adaptation method

At the current stage of work, the considered model is simple, but the full task of the inherent stress modeling process will be much more computationally expensive, therefore, mesh adaptation added to reduce the computational costs. Mesh adaptation allows to reduce computational cost, to correct mesh in complex areas or areas of high gradients. For mesh adaptation, we used the method previously used in [8, 9]. This method based on discretization matrix eigenvalues estimation.

Initially, uniform finite volume mesh was generated (figure 2). Elements type – hexahedra. Then the mesh was adapted. This mesh adaptation process included the following steps:

1. Discretization matrix \( \mathbf{A} \) generation.
2. Scalar field \( \mathbf{F} \) generation, which based on matrix \( \mathbf{A} \) eigenvalues estimation with Gershgorin circle theorem.

\[
f_i = |a_i| + \sum_{i \neq j} |p_{ij}|
\]  

(1)

3. Scalar field \( \mathbf{F} \) normalization.
4. Mesh adaptation – cells refinement or merging, based on $F$ field values.

\[
\begin{align*}
    f_i \text{ normalized} = \frac{f_i}{\max(f)} \\
    f_i \begin{cases} 
        \geq \text{thresold}, & \text{refine} \\
        < \text{thresold}, & \text{merge}
    \end{cases} 
\end{align*}
\]

Experimentally, the threshold was chosen $\text{thresold} = 0.4$.

The initial finite-volume mesh contains 4050 elements. After the refinement finite-volume mesh contains 10000 elements. This maximum number of elements was fixed during remeshing algorithm.

7. Temperature distribution in the molten bath. Simulation results

OpenFOAM results show enough proper agreement with the COMSOL model [1] results. Parameters such as molten bath length and maximum temperature were compared (see Table 2). The difference between in Molten bath length is 15%.

It is assumed that in order to fully melt an alumina particle, the maximum temperature induced by the laser radiation should be higher than the melting point of alumina ($2040^\circ$ C), but the calculation model does not take into account the melting process.
Table 2. Results comparison.

| Value name                  | COMSOL model | OpenFOAM model | Difference (COMSOL=100%) |
|-----------------------------|--------------|----------------|--------------------------|
| Molten bath length, [µm]   | 165          | 190            | +15%                     |
| Maximum temperature, [°C]  | 3380         | 3000           | -11%                     |

Figure 4 shows the OpenFOAM simulation results, figure 5 shows the simulation results of COMSOL [1]. These differences are caused by the different implementation of computational models in OpenFOAM and in COMSOL. In particular, the fact that the heat transfer coefficient between the environment and the powder bed in OpenFOAM solver was assumed to be constant and independent of temperature. In this modeling was not taken into account the compression and expansion of the material during melting and solidification were done — this will be done in the subsequent work.

Figure 5. COMSOL laser convention simulation [1]. Temperature distribution (°C).

Figure 6 shows the comparison of the Temperature residuals for the cases of a uniform and refined mesh. The residual graph in the case of a uniform mesh is, as expected, above the residual of adapted mesh case. In the current modeling task, the computational complexity in the case of adapted mesh is higher than in the case of uniform mesh, since adapted mesh has more finite volumes – cells. But at subsequent stages of 3D-printing modeling, where the computational model will be more complicated and more refined mesh will be required – adaptive mesh will benefit not only in the accuracy of the calculation but also in problem computational complexity reduction.
8. Conclusion
Thermal simulations of the SLM were carried out. The current work shows a good agreement between the results obtained during the simulation in OpenFOAM and COMSOL-based model [1]. Note that the results of the work [1] showed proper agreement with experimental results. Mesh adaptation allowed to increase the convergence of the problem.

The OpenFOAM solver and example are available on GitHub [10] and can be used for further residual stresses model development.

9. References
[1] Peyre P, Aubry P, Fabro R, Neveu R and Longuet A 2016 Analytical and numerical modelling of the direct metal deposition laser process Journal of Physics D: Applied Physics 41(2) 025403 DOI: 10.1088/0022-3727/41/2/025403
[2] Han Q, Setchi R, Evans S and Qiu C 2016 Three-dimensional finite element thermal analysis in selective laser melting of Al-Al2O3 powder Solid Freeform Fabrication 2016: Proceedings of the 27th Annual International Solid Freeform Symposium
[3] Labudovich M, Hu D and Kovacevic R 2003 A three dimensional model for direct laser metal powder deposition and rapid prototyping Journal of Materials Science 38 35-49
[4] Han Q, Setchi R and Evans S 2016 Synthesis and characterisation of advanced ballmilled Al-Al2O3 nanocomposites for selective laser melting Powder Technol. 297 183-192
[5] Khaimovich A, Stepanenko I and Smelov V 2018 Optimisation of Selective Laser Melting by Evaluation Method of Multiple Quality Characteristics IOP Conference Series: Materials Science and Engineering 302(1)
[6] Khairallah S, Anderson A, Rubenchik A and King W 2016 Laser powder-bed fusion additive manufacturing: Physics of complex melt flow and formation mechanisms of pores, spatter, and denudation zones Acta Mater. 108 36-45
[7] Holzmann T 2019 LASER Convection BC URL: http://voluntary.holzmann-cfd.de/publications/laser-convection-bc
[8] Avdeev E, Volkova K and Ovchinnikov V 2017 Final drive lubrication modeling Trudy ISP RAS 29(6) 321-330
[9] Avdeev E, Fursov V and Ovchinnikov V 2015 An adaptive mesh refinement in the finite volume method CEUR Workshop Proceedings 1490 234-241
[10] LaserCase OpenFOAM 2019 URL: https://github.com/j-avdeev/LaserCase

Figure 6. Comparison of Residuals for Temperature for uniform and adapted mesh cases.
Acknowledgments
The author would like to thank Aleksander Khaimovich and Anton Agapovichev for consultation, Tobias Holzmann for the developed and shared the laserConvBC library.