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New data perspective for selective laser melting simulations

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In selective laser melting (SLM), a powdered material is locally melted by a laser and, after cooling, forms a coherent solid structure that enables the production of complex geometries with various materials. The process involves extreme heating and cooling rates and, thus, large temperature gradients, which lead to anisotropic material properties on the macroscopic scale and, in the worst case, reduced mechanical properties. In order to reliably predict the final mechanical component properties, simulations can be performed at different time and length scales. Enormous computational resources are often required to perform such simulations. In order to transform these simulations into suitable surrogate models, the generated data must be compressed and evaluated in a suitable way. This paper shows first preliminary work and a possible new data description of such simulations.

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1 **Motivation**

In selective laser melting (SLM), a powdered material is locally melted by a laser and, after cooling, forms a cohesive solid structure that enables the fabrication of complex geometries [1], which is illustrated in Fig. 1. The process involves extreme heating and cooling rates and, thus, large temperature gradients, which can lead to defects, such as pores and cracks [2]. Typical defects, as spherical pores, but also the so-called keyhole effect and lack of fusion, which represents the respective extremes for too much or too little laser power, can significantly lower the mechanical component properties. In order to predict the component material properties, the solidification of the melted powder have to be simulate. In most cases, these simulations are fluid mechanics calculations in which the interaction of the powder with the laser is very accurately and locally resolved [3]. Such simulations are often very computationally intensive and therefore cannot be solved with conventional personal computers. Remedy can be provided by surrogate models generated from result data of previous simulations [4]. However, in order to generate an efficient surrogate model, the data must first be explicitly selected, evaluated and processed. This paper deals with the postprocessing of SLM simulation data from fluid mechanics simulations to generate surrogate model that can qualitatively represent the defects on the powder scale.



Fig. 1 Illustration of SLM process at macro scale and typically associated SLM defects on powder scale.

2 Simulation data

To build the surrogate model with simulation data from an SLM process, we performed fluid mechanics simulations for a small area of a powder bed melted with a laser and subsequently solidified. The simulation on the powder scale is realized by

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the icoReactingMultiphaseInterFoam solver (iRMIF) from the open source software OpenFOAM [5], which solves a single momentum equation of phases mixture by using the Volume Of Fluid (VoF) method. Through the VoF method, multiple phases including the interfacial change is capture. The mapping of the phases in a cell is done by the phase concentration C, which can be in the range between 0 and 1. Here C = 0 indicates 100% phase-1 (no material) and 0% phase-2 (material), and C = 1 corresponding vice versa. A phase concentration in between indicates a mixture and the interface between the two phases, as illustrated in Fig. 2. Filtering the phase concentration field with a threshold value of C = 0.5 provides the corresponding microstructures of the solid phase, exemplified in Fig. 3.

0.	0.	0.	0.	0.
0.7	0.3	0.01	0.	0.
1.	1.	0.6	0.01	0.
1.	1.	1.	0.2	0.
1.	1.	1.	0.6	0.

Fig. 2 Principle of the Volume of Fluid method: Gray and white fields indicate phase-1 and phase-2, respectively.



Fig. 3 Result of SLM fluid mechanics simulation: resulting microstructure for two different timesteps with threshold C = 0.5.

The phase field in Fig. 2, which is filled with many zero values (no material), is clearly visible. Out of this observation arose the effort to find a possible alternative data representation, which enables to easily characterize and interpret an existing phase concentration field without storing all zero values. A very effective method for data compression while keeping the compressed data interpretable for images are histograms [6]. Generally, the statistical frequency of gray or color values of pixels can be determined and displayed in a histogram. The simulation data should now similarly be displayed and examined.

3 Description of the phase field with histograms

The goal of the surrogate model is to store the area of one of the two phases (in the following, phase-1, no material) not in three-dimensional space, as provided by the SLM fluid mechanics simulation, but with a histogram in each direction. At the same time, information about the position and material fraction of the pore should be preserved and interpretable. To transfer the 3D simulation data into three histograms the following steps are necessary, as illustrated in Fig. 4:

- 1. Cut of the 3D phase field into slices along the coordinate axes
- 2. Sum the pixel values of each slice for x, y, z direction and process the three slices:
 - (a) thresholding the slice with $C \le 0.5$
 - (b) counting the occupied cells
 - (c) generate histograms with bin numbers equal to pixel number.
- 3. Display the three histograms for x, y, z direction.



Fig. 4 Illustration of the three steps to display the 3D phase field by histograms, using a double cone-shaped pore as example.

3 of 6

As a result, three phase distributions are obtained. In the case of a 3D phase field of size $N \times N \times N$, the dataprocessing results in three distributions of the size N, one for each spatial direction. This corresponds to a significant data reduction from N^3 to 3N values that have to be stored. Even though this procedure is straight-forward, often the exchange of result data from the simulation program to the development environment is complex. In the present case, the exchange was realized via CSV data from Paraview [7], which can be handle by the most programming languages, in our case the Julia Programming Language [8].

4 Postprocessing of synthetic and simulated pores

In the following, SLM-typical defects and associated phase fields are converted into histograms using the procedure introduced above. For this purpose, synthetically generated phase fields with one cuboid, several distributed spherical pores, and once keyhole pore originating from a OpenFOAM simulations are evaluated. Fig. 5 to Fig. 7 show, the corresponding phase fields, on the left and the resulting histograms along the x, y and z direction on the right.



Fig. 5 Phase field and histograms along the x, y, and z direction for a cuboid pore.

For a single pore, as in the case of the cuboid and keyhole pore in Fig. 5 and Fig. 7, characteristic profiles for all spatial directions are well recognizable. Thus, even through the highly compressed representation using histograms, the pore type can be identified. In contrast, the phase field of several spherical pores leads to complex histograms, as Fig. 6 shows, because the projection in axial direction causes superpositions of the pore domains, whereby individual pores can no longer be represented separately with the reduced data description. What can be evaluated, however, is the distribution of the pores and their material fraction, which is usually sufficient for the evaluation of SLM simulations results.



Fig. 6 Phase field and histograms along the x, y, and z direction for multiple spherical pores.



Fig. 7 Phase field and histograms along the in x, y, and z direction at a keyhole pore.

5 of 6

5 Conclusion

In this paper a new procedure for the postprocessing of SLM simulation data from fluid mechanics simulations is presented. The basic idea is to qualitatively map the phase fields by characteristic histograms with respect to SLM-typical defects like spherical or keyhole pores. Besides a high data reduction, the presented procedure can also be used to create a surrogate model. A first study with synthetic and simulated pores were performed using the new procedure. For single pores characteristic histograms are be generated, from which the pore location, shape and the material fracture can be evaluated. If several pores are located in one area, individual pore properties can no longer be evaluated when creating the histograms due to pore overlaps. However, the material proportion and the distribution of the pores can still be evaluated, which allows statements about the quality of the SLM component produced. In the future, besides qualitative features, also quantitative features shall be considered. Furthermore, this representation of data can be used advantageously in algorithms with neural networks to fastly analyze phase field data.

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