Solid Freeform Fabrication 2024: Proceedings of the 35th Annual International
Solid Freeform Fabrication Symposium – An Additive Manufacturing Conference
Reviewed Paper

DEEP LEARNING BASED PREDICTION OF THERMAL HISTORY DURING THE LASER-BASED POWDER BED FUSION (PBF-LB) ADDITIVE MANUFACTURING PROCESS

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Abstract

Laser-Based Powder Bed Fusion (PBF-LB) is a key technology in additive manufacturing (AM) for metals, offering a high degree of design freedom for complex geometries. Accurate modeling of the thermal history and resulting material properties is critical, especially for steels with solid-state phase transformations. This research integrates high-fidelity multi-scale finite element method (FEM) simulations and long-short term memory recurrent neural networks (RNN-LSTM) to efficiently predict thermal histories. The RNN-LSTM model, trained on FEM-generated data, demonstrated high prediction accuracy for demonstrators of different sizes. The performance of the model was trained and evaluated for three datasets, with the steady-state dataset yielding the highest prediction accuracy. This approach can improve material characterization in PBF-LB, optimize printing strategies, and elucidate the relationship between process parameters and the resulting microstructure.

Introduction

Laser-based powder bed fusion (PBF-LB) process has become one of the standard additive manufacturing (AM) processes for metals. This process has several key advantages such as a high freedom of design for complex geometries that would be difficult or impossible to manufacture with conventional manufacturing methods. Due to the highly localized energy input of the laser system, the resulting material properties are strongly influenced by the used parameter set and processing strategy (Damon et al., 2019; Kürnsteiner et al., 2020; Schüßler et al., 2023). This is aspect especially important for materials with solid-state phase transformations such as maraging and quench and tempering steels as the phase transformations can lead to significant variability of material properties. Therefore, a localized variation of processing parameters and processing strategy shows the possibility to create functionally graded materials (FGMs) directly within the process, removing the need of a subsequent heat treatment to reach locally optimized material properties.

In order to use the full potential of the PBF-LB process and locally adjust the material parameters, the process parameters and processing strategies have to be characterized and optimized. Such a process is often done by a time-consuming experimental trial and error method. A recent approach in the literature is to use FEM simulations in order to predict the thermal history and therefore the resulting material properties. The use of FEM simulations is well established for materials without a solid-state phase transformation such as austenitic steels (Bellet et al., 2023; Williams et al., 2018). The accuracy needed to model the solid-state phase transformations for maraging or quench and tempering steels significantly increases the computational cost due to the smaller time increments and spatial resolution needed to model these transformations. The authors recently proposed a multiscale FEM simulation framework for materials with solid-state phase transformations that significantly reduces the computational cost while maintaining a high accuracy (Schüßler et al., 2023). While this approach makes a part scale simulation possible, the simulation times are still in the range of hours to days.

An interesting method to significantly reduce the computational cost are deep learning based methods. Generally, these deep learning methods need data in order to train a mathematical model, the model can then be used to predict the results for similar datasets with minimal computational cost (likely less than one second for a prediction).

Different models have been used to classify defects or predict material properties and surface roughness by the use of experimental training data (Bordekar et al., 2023; Poudel et al., 2022). While these models can predict these properties with a high accuracy, the training data is time-consuming to measure and analyze. Multiple publications therefore highlighted the possibility of the combined usage of validated FEM simulations with deep learning based methods. The FEM-simulation is therefore used to generate the labels for the training, testing and validation of the deep learning based methods. Multiple different deep learning methods were used such as simple feed-forward neural networks (FFNN), physics informed neural networks (PINN), convolutional neural networks (CNN) or recurrent neural networks (RNN) (Ahmed et al., 2023; Le et al., 2023; Peng and Panesar, 2023; Pham et al., 2023; Yi et al., 2022).

The objective of this research is to use the high-fidelity temperature history calculated by the multiscale FEM simulation (Schüßler et al., 2023) to train a Long-Short Term Memory recurrent neural network (RNN-LSTM) (Gers et al., 2000; Hochreiter and Schmidhuber, 1997) with the goal to use only a few sub part-scale FEM simulations to predict bigger parts. The prediction quality was then analyzed for the extrapolation for more layers or bigger parts. The extrapolation is therefore validated by the thermal history calculated by the multiscale FEM simulation. There are two main dimensions for extrapolation: higher parts or parts with a higher cross sectional area. Due to the constraints of these publications the authors only focused on the extrapolation to higher parts, therefore more layers of the same cross section. The outcomes of this investigation will enhance the characterization of material properties of PBF-LB, aiming to enhance the efficiency of single and multi-parameter printing strategies and elucidate the correlation between tempering states and various combinations of process parameters.

Methods

In order to predict the thermal history for the PBF-LB process the process parameters and the processing strategy have to be known at each time step of the process. Therefore, the Autodesk Netfabb slicer was used to slice the parts and create a machine readable output file which includes all necessary information about the process. The sliced strategy data was further analyzed by a python script in order to extract the process data for each time step (e.g. current laser power, current scan speed, current laser position).

First, the process data was used to calculate the thermal history with a high-fidelity multiscale FEM simulation (Schüßler et al., 2023) in order to generate the training data for the deep learning model. The FEM simulation was created and validated in a previous publication (Schüßler et al., 2023). The validated FEM models were used for this study as indirect validation since the

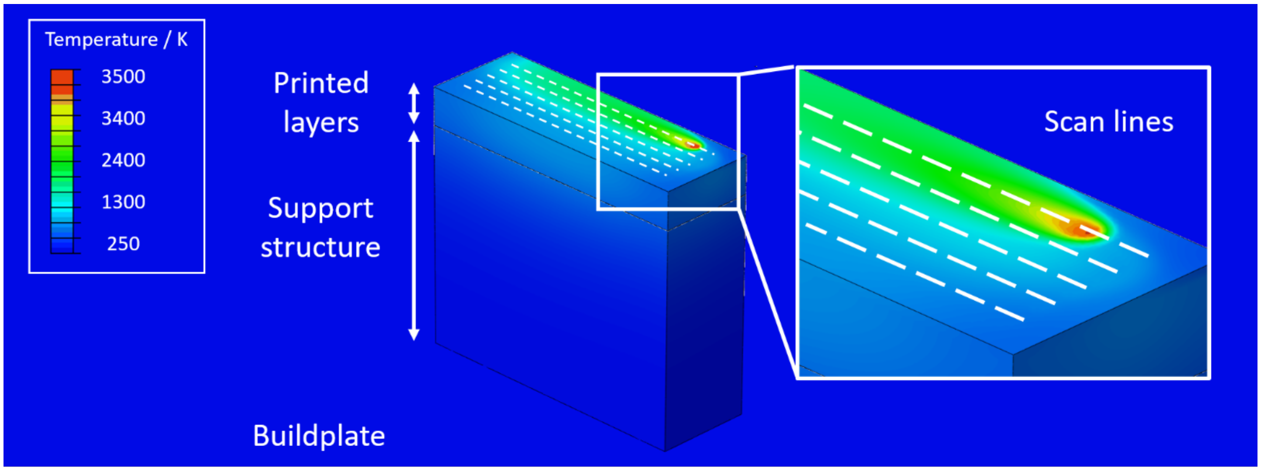

Figure 1 Exemplary visualization of the thermal gradients calculated by the multiscale FEM simulation during the printing process. The printed part has a surface area of about 1.0 mm² with a scan line length of 2 mm and 5 subsequent scan lines per layer and was used as part of the training dataset.

direct validation with measured temperature data is not possible. The thermal history for each selected node was automatically analyzed and exported. The variable sequence length of the FEM simulation was interpolated to a fixed sequence length of $1*10^{-4}$ s for use with the deep learning model. Multiple FEM simulations with different part sizes were calculated, analyzed and exported to form the dataset (Cross sectional area from 0.5 mm² to 4 mm², Figure 1). Three datasets were created for the training and one dataset for the validation: A high-temperature dataset containing the sequential data for the first three layers, a transition dataset containing the sequential data for the first five layers, a steady-state dataset containing the sequential data for the first seven layers and an extended steady-state dataset containing the first ten layers for validation of the extrapolation. The high temperature dataset included the thermal history for 3128 nodes with 2001 time steps each, resulting in a total of 6.25 million data points. The transition dataset included the thermal history for 3128 nodes with 5001 time steps each, resulting in a total of 15.64 million data points. The steady-state dataset included the thermal history for 3128 nodes with 7001 time steps each, resulting in a total of 21.90 million data points. The extended steady-state dataset for validation included the thermal history for 3128 nodes with 10001 time steps each, resulting in a total of 31.28 million data points. The selected nodes are homogeneously distributed inside the respective layers.

Secondly, the generated process data used to create the FEM simulations was also used as the input of the deep learning neural network. The process data was further analyzed in order to calculate the 12 features used for the proposed model. These features include the current laser power, scan speed, the scan line progress, as well as the relative distances between the node and the start of the scan line, the node and the end of the scan line and the node at the current laser position for all three dimensions. The relative coordinate system for the scan lines was chosen in order to avoid data augmentation to represent rotated or translated process data. The 12 features were then scaled to values between zero and one, dependent on the maximum and minimum value of each type. As the deep learning model should be able to predict the thermal history, a recurrent neural network (RNN) model designed for sequential data was selected for this study. More specifically the optimized architecture of the Long-Short Term Memory (RNN-LSTM) model was used (Gers et al., 2000; Hochreiter and Schmidhuber, 1997) for improved prediction accuracy. The

RNN-LSTM model was implemented with python and the PyTorch package (Paszke et al., 2019). After optimization, the model used 32 hidden nodes with 4 layers, a learning rate of $1*10^{-3}$ and a batch size of 100 nodes. The complete dataset was split into two sub-datasets for training (50%) and testing (50%). The loss was calculated by the mean squared error (MSE) function for each epoch. The temperature history calculated by the FEM simulation was used as a reference during the training, testing and validation phases.

Results and Discussion

To train, test, and validate the RNN-LSTM model, the previously validated multiscale FEM simulation framework was used (Schüßler et al., 2023). Figure 2 shows an example thermal history of a single node extracted from the FEM simulation. The temperature profile reveals temperature peaks during the laser processing of each layer, as well as the rapid cooling during the pause or recoating between the processing of each layer. A global trend of a decreasing peak temperature is seen as more layers are added, resulting in a slightly decreasing peak temperature of less than 700 K after 6 layers. The computational time for one small-scale FEM simulation was between 4 h (3 scan lines with 1 mm each) and 25 h (5 scan lines with 2 mm each) with the author's workstations.

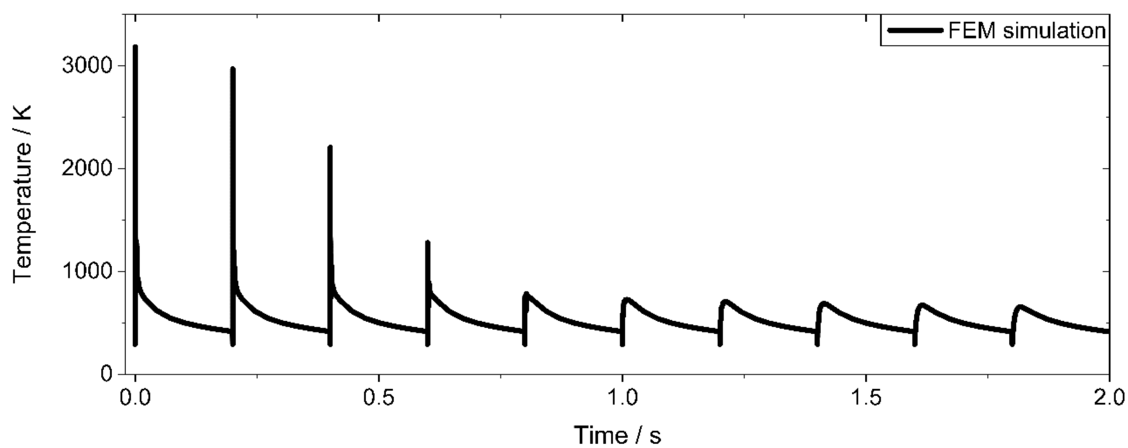

Figure 2 Exemplary thermal history for a node of the extended steady-state validation dataset.

High-temperature dataset

The first part of the study used the small dataset with sequential data for the first three layers. Since the peak temperature during the processing and the subsequent melting of the material occurs while processing these layers, the respective dataset mainly contains high-temperature training data. This dataset was used during the training, testing and validation phase of the RNN-LSTM optimization. Figure 3 (left) shows the evolution of the thermal history prediction during the training phase of the data point with the highest resulting MSE-loss. This data point was part of the validation dataset. A steady improvement for the thermal history prediction is seen from the first to the last epoch. A similar improvement of the model prediction accuracy is also visualized by the MSE-loss curve in Figure 3 (right). A steady improvement is noted for the first 10000 epochs, with significantly lower improvement afterwards for both the MSE-loss on the training and testing dataset. In order to characterize the ability of the trained model to generalize, the model was evaluated with the extended-steady-state dataset (Figure 4). The model is able to accurately predict the thermal history for the first three layers for which training data existed. The quality of prediction for any further layers is twofold. The trained model is able to predict the repetitive heating and cooling cycles during the PBF-LB process for multiple layers, while significantly overestimating the peak temperatures for every extrapolated layer.

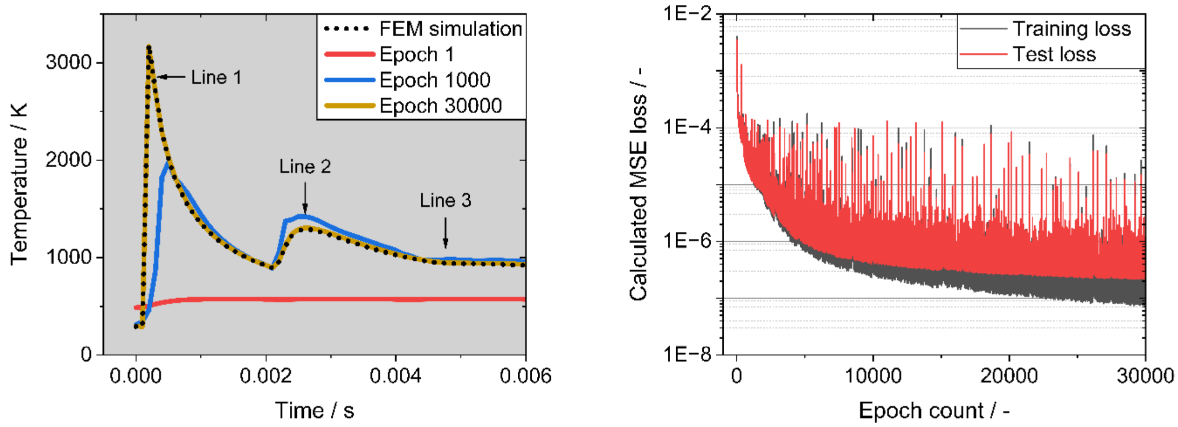

Figure 3 The evolution of the predicted thermal history for the first layer during the training process with the high-temperature dataset (left) and the corresponding training and test loss (right).

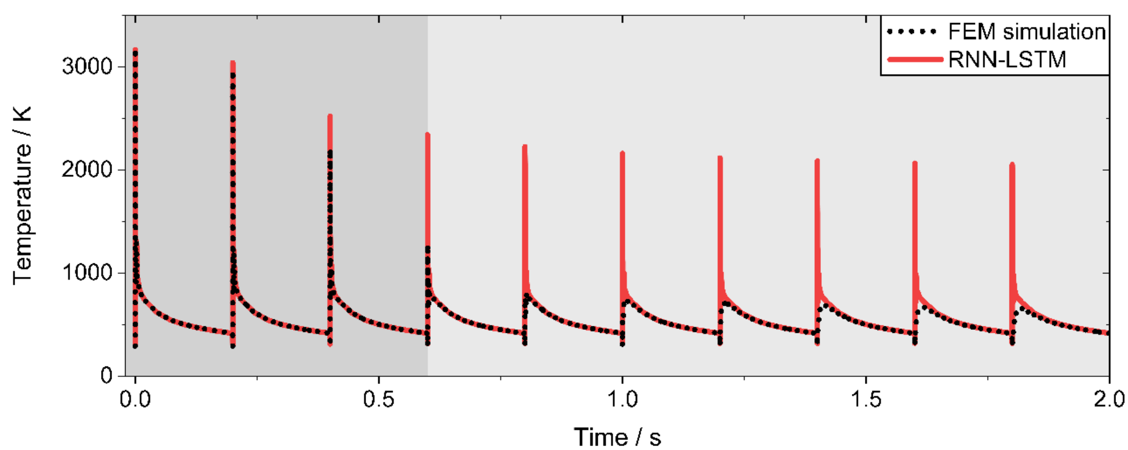

Figure 4 Predicted thermal history for the model trained by the high-temperature dataset. FEM simulation data from the zone with the dark grey background was used for the training of this model (interpolation), while the model never used data from the zone with the light grey background for training (extrapolation).

Transition dataset

A similar study was conducted for the transition dataset. The trained model is also able to accurately predict the thermal history for which training data existed. Figure 5 (left) shows the predicted thermal history for the first layer of the data point with the highest MSE-loss of the extended-steady-state dataset. The loss curve during the training process looks slightly different compared to the high-temperature dataset with a small plateau due to a local minimum, which could be avoided with further training epochs (Figure 5 (right)). The loss after the training was completed was similar to the high-temperature dataset. The model trained on the transition dataset is able to predict the thermal history of the bigger extended-steady-state dataset with a significantly higher accuracy when directly compared to the high-temperature dataset (Figure 6). The model is able to predict the cyclic heating and cooling intervals as well as the decreasing peak temperature during the transition phase. Constant peak temperatures of the extrapolated layers were noted for the prediction while the FEM-simulation shows a slightly decreasing peak temperature if more layers were printed on top of the sample.

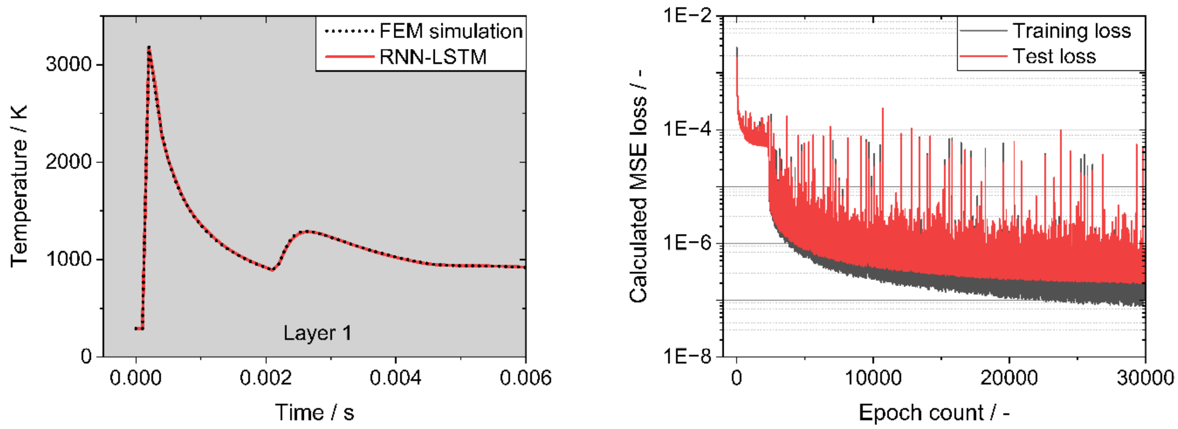

Figure 5 The predicted thermal history for the first layer after the training process with the transition dataset (left) and the corresponding training and test loss during the training phase (right).

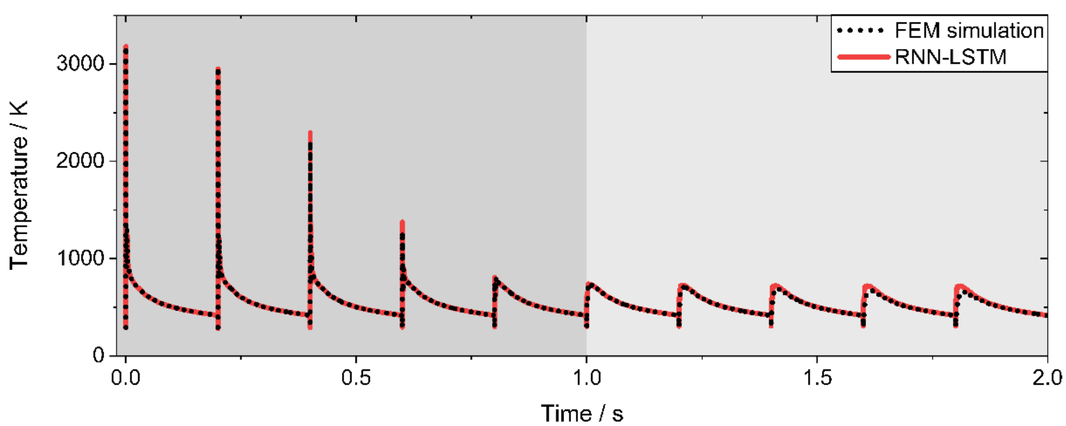

Figure 6 Predicted thermal history for the model trained by the transition dataset. FEM simulation data from the zone with the dark grey background was used for the training of this model (interpolation), while the model never used data from the zone with the light grey background for training (extrapolation).

Steady-state dataset

The third dataset used the sequential data for the high-temperature, transition and steady state region for the training process of the model. The model trained subsequently is also able to predict the thermal history of the first layer with high accuracy as Figure 7 (left) shows the data point with the highest resulting MSE-loss of the dataset. The MSE-loss curve during training shows a rapid improvement for the first epochs with a resulting MSE-loss slightly lower compared to the other two used datasets (Figure 7 (right)).

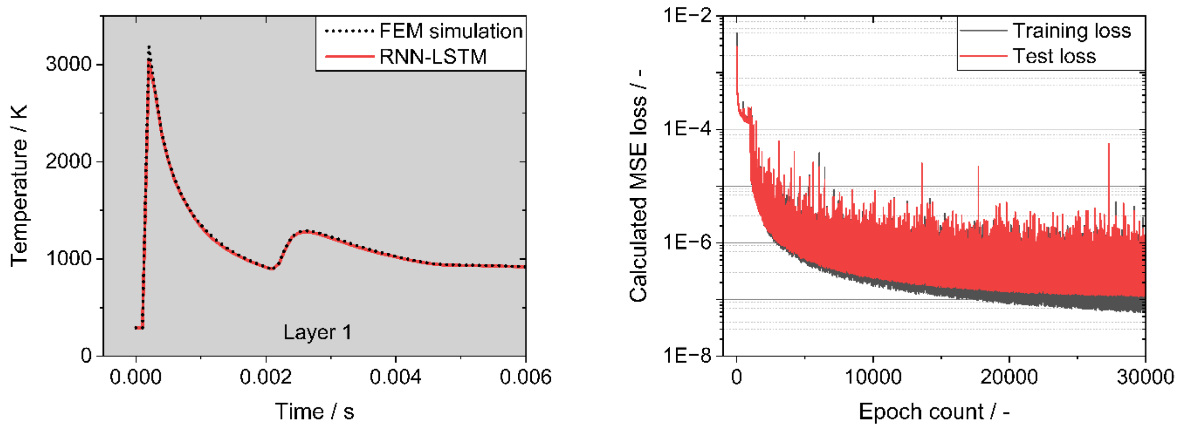

Figure 7 The predicted thermal history for the first layer after the training process with the steady-state dataset (left) and the corresponding training and test loss during the training phase (right).

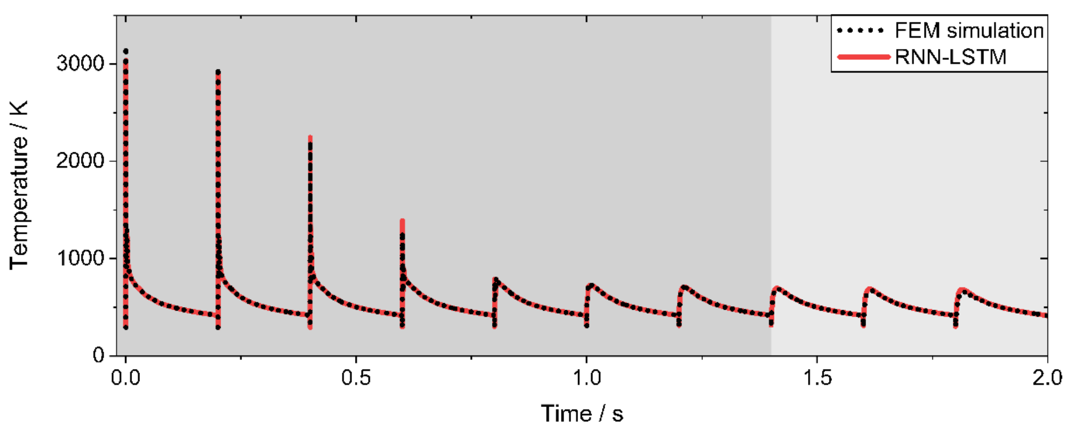

Figure 8 Predicted thermal history for the model trained by the steady-state dataset. FEM simulation data from the zone with the dark grey background was used for the training of this model (interpolation), while the model never used data from the zone with the light grey background for training (extrapolation).

The trained model is also able to predict the thermal history of the extended-steady-state dataset with the highest precision of the three implemented datasets (Figure 8). The model improves the prediction of the extended-steady-state dataset regarding the peak temperatures for the extrapolation to additional layers. These results highlight the robustness and adaptability of the model across different thermal histories, demonstrating its potential for various applications in thermal management and predictive maintenance. The lower MSE loss achieved with the third data set suggests that incorporating sequential data from different thermal states significantly improves the model's performance, making it more reliable for practical use. In addition, the ability to accurately predict thermal history and peak temperatures is critical for optimizing manufacturing processes, such as additive manufacturing, where precise thermal control can lead to improved material properties and reduced defects. The success with the steady-state data set also suggests that the model can be extended to predict the behavior of full sized parts. The new method is also able to reduce the computational cost for the prediction. While the input data generation took up to

25 h, the training was completed in under 5 h and the predictions with the trained model take less than a second.

Conclusion

This study successfully uses the results of a few selected multiscale FEM simulations as training data for a recurrent neural network (RNN-LSTM) in order to predict the thermal history of PBF-LB processes. The following conclusions can be drawn from this study:

- Reduced computational cost: The integration of FEM simulation and RNN-LSTM models significantly reduces computational cost and time, making part-scale simulation of materials with solid-state phase transformations more feasible.
- High prediction accuracy: The RNN-LSTM model accurately predicts thermal histories, especially when trained with larger data sets, improving the reliability of simulations.
- Extrapolation: The models trained with a transition or steady-state dataset successfully predicted the thermal histories for higher parts, than the model used during the training process (extrapolation).
- Optimized printing strategies: This approach enables a more efficient parameter optimization for the PBF-LB process, supporting the development of functionally graded materials and better control over resulting material properties.

Further research should be centered around the extrapolation to bigger cross sectional areas and for multiple process parameters. The main goal will be to minimize the training dataset, while still enabling the model to generalize to different parts and processing strategies.

Acknowledgment

This research was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – grant number 516837935.

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