Supplementary Information:
Mechanical Behavior Predictions of Additively Manufactured Microstructures using Functional Gaussian Process Surrogates

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1 The features demonstrated by the training set RVEs as well as the 300 grain RVEs shows features akin
2 to those seen in single track AM experiments [1]. However, in general, the AM process involves continued
3 melting and re-solidification of the metal powder as well as previously built layers. This results in grain
4 formation that expitaxially grow competitely according to the thermal gradients of the melt pool. There are
5 a number of ways to approach modeling the microstructure formation phenomenon [2]. The least physical
6 approaches are purely statistical methods based on simulating the parameters of a tessellation model, with the
7 drawback that these models are too simplistic to capture the complex morphologies of AM microstructures.
8 The CDIM used in this work incorporates a slightly higher fidelity than these methods but is limited to grain
9 growth along specific axes. The highest fidelity models incorporating the most realistic physical phenomena
10 are phase field models that incorporate the kinetics of microstructure evolution into an energy functional to be
11 minimized. While this approach enables studying effects of competing mechanisms, it is too computationally
12 demanding to simulate large polycrystalline microstructures. The cellular automata finite element (CAFE)
13 model is a popular technique to simulate microstructure solidification because of its relationship between
14 computational tractability and fidelity of physics [3, 4]. In the CAFE model, the heat equation is solved
15 based on the laser scan history to compute the temperature field and its gradient during microstructure
16 evolution.

17 In this work, a CAFE model that has been modified to optimally simulate the solidification of AM metals
18 in large domains (on the order of 0.5-1 cm^3) is implemented for the generation of a microstructure to evaluate
19 the fGP framework. In this model, the small time scale of the solidification analysis is treated independently,
20 as sub-cycles, within each larger scale discrete time step associated with the temperature field. Additionally,
21 rather than growing the solidification front by using very small time steps in each sub-cycle, the time it takes
22 for each solid voxel to capture its neighboring voxels is predicted and the simulation evolves sequentially
23 based on priorities associated with the estimated time of capture. An additional modification to the CAFE
24 model, which improves computational efficiency, is the determination and consideration of only the current

₂₅ active region(s) in the domain, which for AM is the region of the heat affected zone where the material is
₂₆ undercooled (*i.e.*, below liquidus temperature) but has yet to be solidified. The CAFE model is used to
₂₇ simulate the epitaxial grain growth from the base plate of the AM build by incorporating empirical models
₂₈ for analyzing competitive growth, such as preferential crystallographic growth or thermal gradient driven
₂₉ growth. An instantiation of the CAFE model consisting of 3 slightly overlapping tracks and multiple layers
₃₀ is shown in supplementary figure 1.
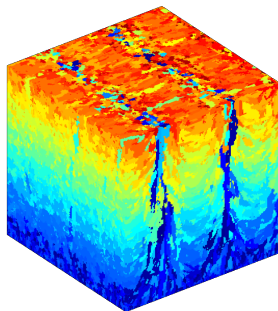
(a)
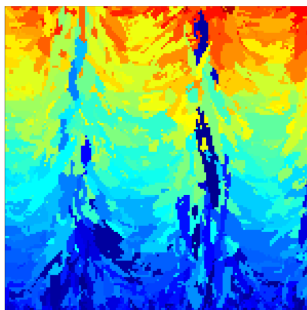
(b)

Figure 1: **Cellular Automata Model.** Polycrystalline microstructure generated using the modified CAFE model. **a.** Full 3D microstructure consisting of 3 tracks and multiple layers. **b.** A 2D cross-section of the same microstructure, which better demonstrates grains growing in the direction of the melt pools. Grain colors correspond to grain labels from 1 to N, where N is the total number of grains.

₃₁ From the microstructure shown in supplementary figure 1a, a smaller RVE ($56.25 \, \mu m^3$) is extracted to
₃₂ evaluate the performance of the fGP network that has been trained on CDIM microstructures. As discussed
₃₃ in the main text, the concept of an RVE in AM is a bit of a misnomer, as clearly there is no truly repeated,
₃₄ representative structure seen in supplementary figure 1. However, an RVE with a representative feature
₃₅ set can be extracted. While the fGP network could be used to analyze the full CA-based microstructure
₃₆ with many thousands of grains, that is not done here. The reason for this being that the fGP network is
₃₇ being evaluated here to assess its performance and limitations on unseen data. This means that whatever is

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chosen to evaluate the fGP network must be able to be simulated using the CPFE model, which is limited
to simulating a few hundred grains. To remove bias, the subset selection is done randomly within the full
microstructure. The chosen RVE and corresponding stress-strain behavior from the CPFE and fGP models
are shown in supplementary figure 2 with corresponding error rates shown in supplementary table 1.
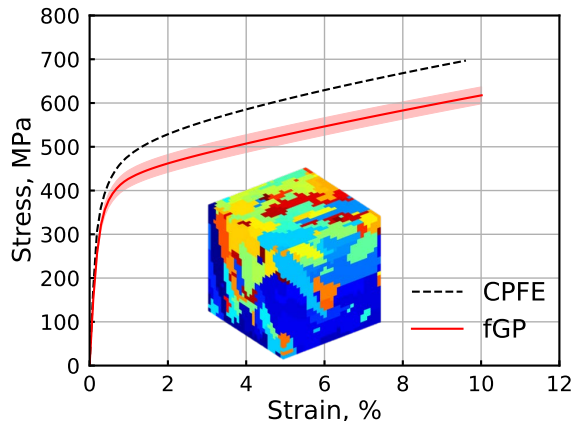

Figure 2: **CA Stress-Strain Results.** Stress-strain data from the CPFE model as well as the fGP graphical
network for the shown RVE that was extracted randomly from the full microstructure of supplementary
figure 1.

Table 1: **CA Data Error Metrics.** Error metrics for the trained fGP strain and stress models on the RVE
extracted from the full CA microstructure.

	MSE	MAE	MAPE	SMSE
Strain	2.002e−4	9.81e−3	29.121%	9.869
Stress	31344.5 MPa^2	113.349 MPa	16.776%	27.079

The results of the fGP network on the CAFE model microstructure are poor and show double digit error
rates, much larger than those seen during training/testing of the model. However, this is not unexpected as
the features seen in the CA-based RVE are significantly different than those seen in the original data set.
As discussed in the main text, the fGP network is a data driven ML model so it can **only** accurately make
predictions on features with similarities to those it has seen before. As can be seen in the CA-based RVE,
the microstructure includes grains which are oriented along many different directions, have many different
aspect ratios, and many different sizes. However, during training of the fGP model, the CDIM was used to
generate microstructures with grains grown along a single RVE axis with different aspect ratios and sizes.

The shortcomings of the fGP network training can be addressed in two ways, both of which will increase
the variety of features in the training data set and make the fGP more applicable to multi-track, multi-layer
AM builds. The first method is to generate multiple (on the order of 10's), large CAFE model microstructures
(as seen in supplementary figure 1) and extract numerous small RVEs, which can then be simulated and

used to retrain or improve the already trained fGP network. This would result in a richer feature set for training and, as a natural consequence of the CAFE model inputs, include AM process parameters in the data generation process. The obvious downside to this method would be the computational expense to simulate the CAFE model many times. Additionally, there is a chance when simulating the CA model that unmelted "powder" can remain in the microstructure, which would need to be removed from the RVEs before simulating with CPFE. The second method, which is conceptually simpler, is to continue utilizing the CDIM but modify the implementation such that grains of varying sizes and aspect ratios can be generated along arbitrary axes within the RVE. The advantage in continuing to use the CDIM is the computational expense, or lack thereof. However, the CDIM will still be an approximation to reality (at a lower fidelity than the CAFE model) and thus may not be preferable if training the fGP network for maximum accuracy on real AM

References

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