

Supplementary Information:

Digitalizing Metallic Materials from Image Segmentation to Multiscale Solutions via Physics Informed Operator Learning

Details on training of the Mask R-CNN

The dataset used for training was generated through phase-field simulations of dendritic growth in a synthetic alloy, with the physical properties detailed in Table S1. The growth process was initiated by a circular seed in a square domain with isolated boundary conditions for the phase field and alloy concentration. The domain measured 1 mm², with a grid spacing of 0.5 μm and an interface thickness of 2 μm . The simulations accounted for latent heat, started under isothermal conditions at 918 K, and included a heat flow of $-100 \text{ J}\cdot\text{s}^{-1}\cdot\text{cm}^{-3}$. Nucleation was randomized following a nucleation density law, and each simulation lasted 10 seconds. Diffusion in the solid phase was not considered. Figure S1a illustrates the dendrite morphology evolution over time in a selected simulation. We can see at 10 seconds that the highest concentration levels are located between the grains. To ensure diversity in the microstructural images, simulations were conducted with varying distributions of initial nuclei. For training the detection model, we used the concentration maps at 10 s from the different simulations. These maps were converted to grayscale to align closely with the gray levels observed in the experimental images, as shown in Figure ???. The higher concentration levels along grain boundaries appear in white, as shown in the Figure S1b.

Table S1: Thermophysical properties of the synthetic alloy inspired by [1].

concentration Cu (c_0) [at.-%]	3
Melting temp. (T_f) [K]	933.5
Liquidus slope (m_l) [K at.-% ⁻¹]	-6
Partition coefficient (k)	0.097
Diffusion coefficient in liquid (D_l) [m ² s ⁻¹]	$3\cdot 10^{-9}$
Diffusion coefficient in solid (D_s) [m ² s ⁻¹]	0
Gibbs-Thompson coefficient (Γ_{sl}) [Km]	$2.36 \cdot 10^{-8}$
Interfacial energy (σ_{sl}) [Jm ⁻²]	$1.6 \cdot 10^{-2}$
Anisotropy of interfacial energy (ϵ_{sl}) [%]	0.1

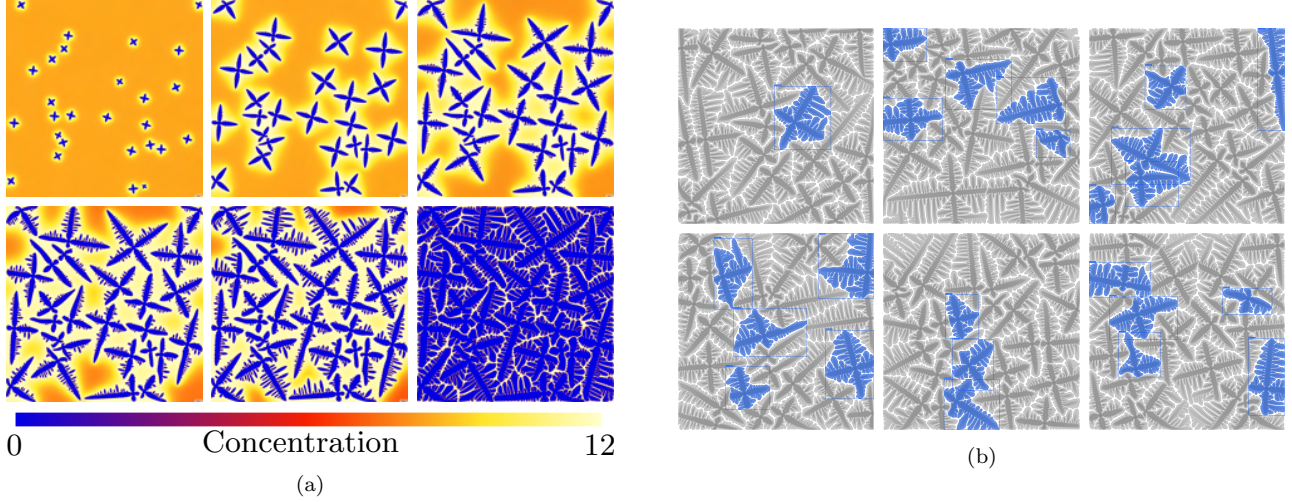


Figure S1: Dendrite morphology evolution. (a) Phase field results at different times of 0.5 s, 1.5 s, 2.5 s, 3.5 s, 4.5 s and 10 s from top left to bottom right. The simulation domain has a size of $0.2 \times 0.2 \text{ mm}^2$ (b) Training image example. Each dendrite is identified by its mask (in blue), generated from phase-field simulations [2].

The training dataset comprises 1,000 images, while the test dataset comprises 100 images with resolutions of 100×100 or 200×200 pixels. Each dendrite in the phase-field simulations was assigned a unique grain number, enabling the generation of direct pixel masks, as shown in blue in Figure S1b. The Mask R-CNN model was implemented using the OpenMMLab [3] framework, with training parameters described in Table S2. The phase-field-generated dataset provided a wide range of dendritic representations, facilitating robust learning.

Table S2: Parameter for the MaskRCNN implemented with Openmmlab [3] (NMS='Non-Maximum Suppression').

Parameter	Value
Number of boxes before NMS:	2000/1000
Number of boxes in NMS	1000
Number of boxes after NMS	1000
IoU threshold	0.9
Threshold for filtering out boxes	0.05
NMS threshold	0.5
Maximum number of detections per image	1000
Mask threshold	0.5
Epochs	30

Morphologies for the 2D FOL model

For the training model we use the following strategy to create the samples. To construct the sample polycrystalline morphologies for the training phase, we utilize the Voronoi tessellation algorithm. When there are no restrictions on periodicity, random locations are assigned for the desirable number of seed points, based on which grain topologies are generated, as illustrated in Fig. S2. The resulting morphology is then meshed using either structblack or unstructblack meshes.

In the FOL framework, the choice of mesh type and boundary conditions is highly flexible, offering significant adaptability to various scenarios. Some of the training samples are

generated based on the parameters reported in Table S3. It is worth noting that light optical microscopy (LOM) or scanning electron microscopy (SEM) images are not necessarily periodic, which motivated us to consider both periodic and non-periodic morphologies in this study.

The dimensions of the volume elements can be set to any desirable value; in our case, we use $50\text{ }\mu\text{m}$, reflecting the typical size observed in the LOM images provided.

Table S3: Parameters used for generating elasticity samples with the Voronoi-based parameterization.

Parameter	Value
Number of seed points M	25
Number of random samples	8000
Number of neurons in the input layer (input features)	25×3
Number of neurons in the output layer (mesh resolution)	11×11 , 21×21 , 51×51

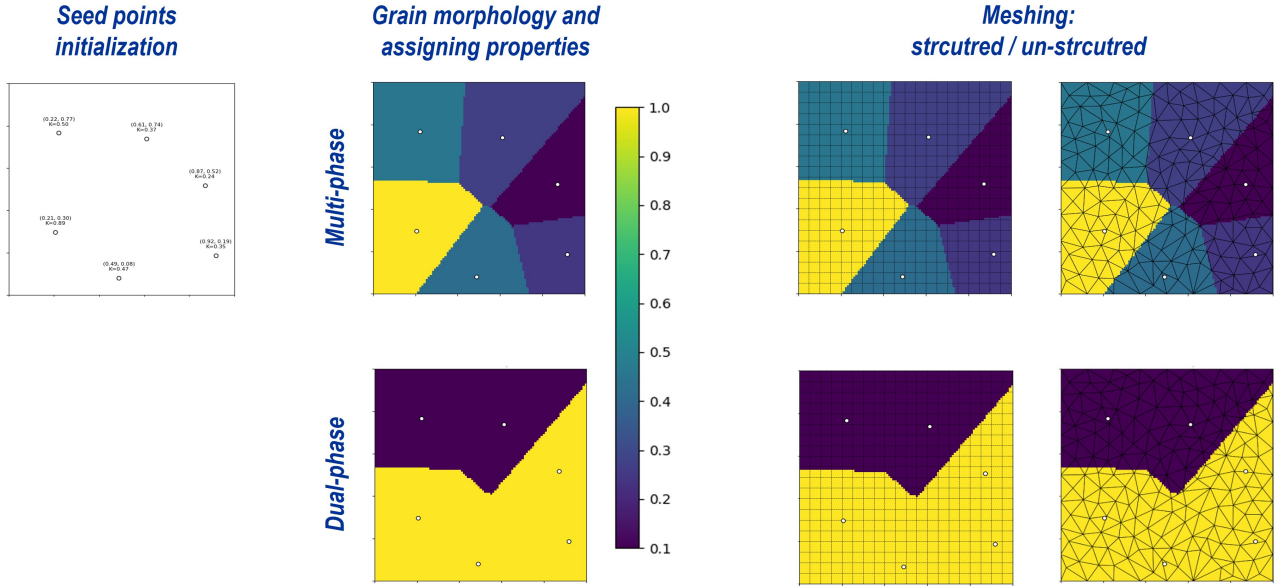


Figure S2: Pipeline for the generation of artificial yet representative volume elements.

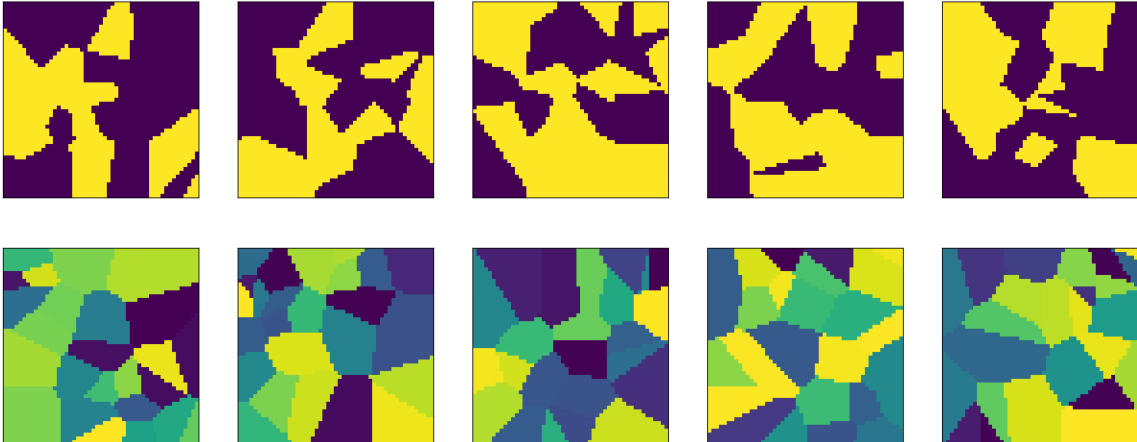


Figure S3: Training samples for FOL model. Dual phase and multi phase polycrystalline microstructure.

Morphologies for the 2D SPiFOL model

The SPiFOL method requires structblack grid points and strictly enforces periodic boundary conditions, making it particularly well-suited for material multiscaling analyses. As discussed, this approach directly pblackicts stress-related quantities, which are especially valuable for multiscale analysis where homogenized properties are the primary focus. For the training phase, we did not feed the network any polycrystalline-shaped microstructures. Instead, we utilized periodic microstructures inspiblack by Fourier-based parameterizations. The equations used to generate these microstructures are provided in Eqs. ???. This approach also allows us to test the extrapolation and generalization capabilities of the model, assessing its performance on unseen periodic polycrystalline microstructures beyond the training data. To further evaluate the SPiFOL performance, periodic polycrystalline microstructures were created and tested. These results are discussed in detail in the “Result” section.

Based on the aforementioned explanations and the parameters outlined in TableS4, we generated a dataset of 8000 samples for training the SPiFOL model. For training the 3D SPiFOL model, the same procedure is used, where only Fourier-based 3D samples are generated to train the network. See [4] and SPiFOL framework.

Table S4: Parameters for sample generation via Fourier-based approach

parameters	values
t_1	$[-1, 0.5, 1, 2, 5, 10, 300]$
t_2	$[0.02, 0.1, 0.5, 1, 2]$
$N_x = N_y$	3
f_x	$[0, 1, 2, 3]$
f_y	$[0, 1, 2, 3]$

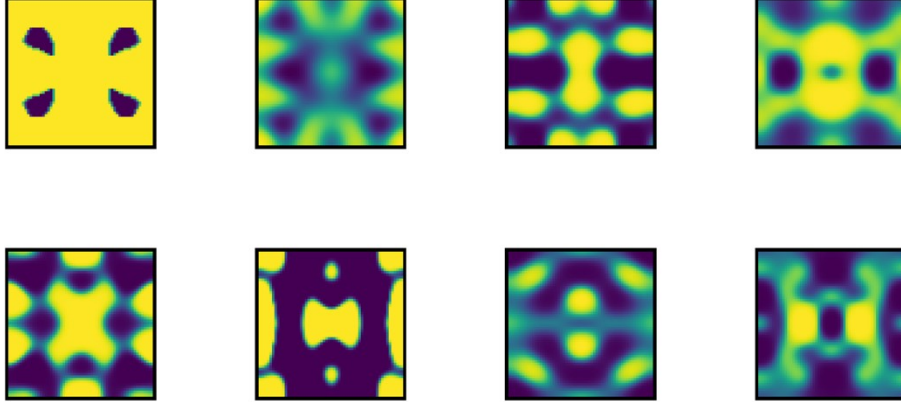


Figure S4: Training samples for SPiFOL model. Randomly selected Fourier microstructures where phase changes from 0 to 1.

Boundary conditions for the 3D FOL model

For the investigations presented in Section “Result”, we varied the components of the applied displacement vector on the front surface according to normalized random distributions. About 1000 samples were created and used for the training, and their distributions are shown in Fig ??. Further details are provided regarding the number of grains (seed points) in the 3D samples and the number of nodes used for the computations. In this framework, the network inputs

are the three components of the applied Dirichlet boundary conditions, denoted by u_1 , u_2 , and u_3 . The histogram of the generated samples is shown in Fig. ??, highlighting the frequency of different input values. Notably, the exact paths of the test cases are excluded from the training data, with some samples intentionally selected to deviate from the average values. This deliberate choice challenges the model’s performance by subjecting it to harder and less common test scenarios.

Table S5: Parameters used for generating random loading path for the 3D calculations.

Parameter	Value
Number of seed points M	128
Number of random samples	1000 (Dirichlet BCs)
Number of neurons in the input layer (input features)	3
Number of neurons in the output layer (mesh resolution)	47,547

Convergence analysis

It is also essential to study the influence of mesh resolution or the number of nodes requiblack to capture an accurate solution. This is achieved by refining the mesh and increasing the number of neurons in the output layer for different mesh resolutions. For illustration, a system of dual-phase polycrystalline material is shown in Fig. S5, where the number of nodes varies from 11×11 to 51×51 . As observed, the deformation results eventually converge, and in all cases, the performance of the FOL closely matches that of FEM.

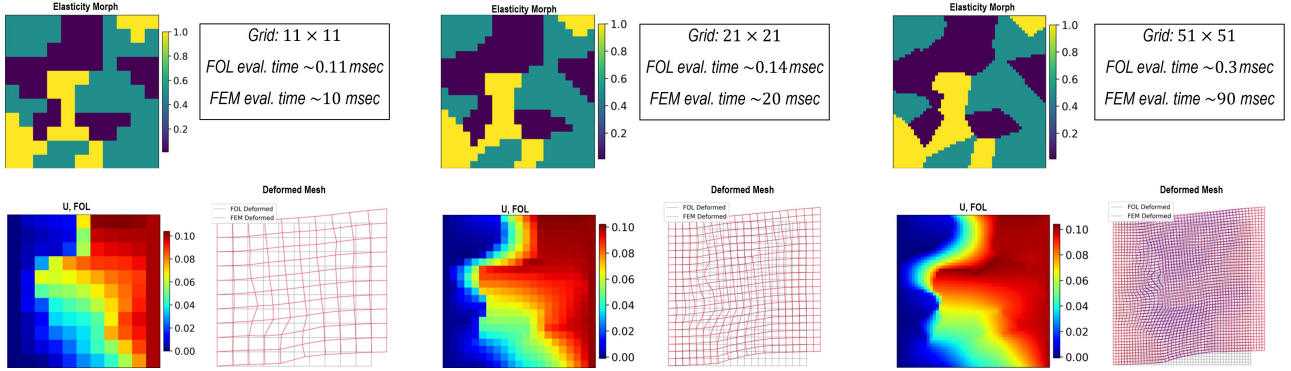


Figure S5: Mesh convergence analysis for the proposed framework.

Interestingly, both training and evaluation times remain nearly unchanged, even with a significant increase in the number of neurons in the output layer, from 121 to 2061. Moreover, we observed a significant blackuction in evaluation costs as mesh density increases. However, it is important to note that we are not claiming this FEM implementation is the fastest available. For the remainder of this study, we will use a 51×51 mesh unless otherwise specified.

Further details on training behavior of the DL models

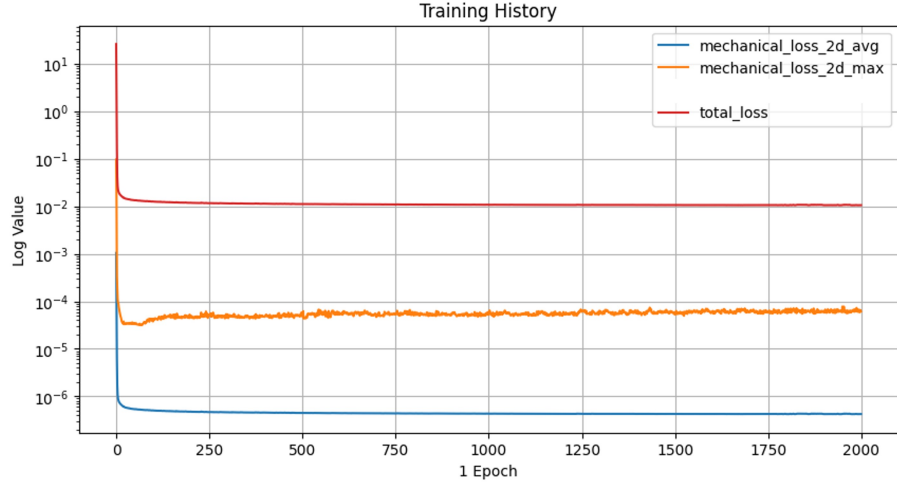


Figure S6: Training history for FOL model. Loss decay and training history for the FOL framework.

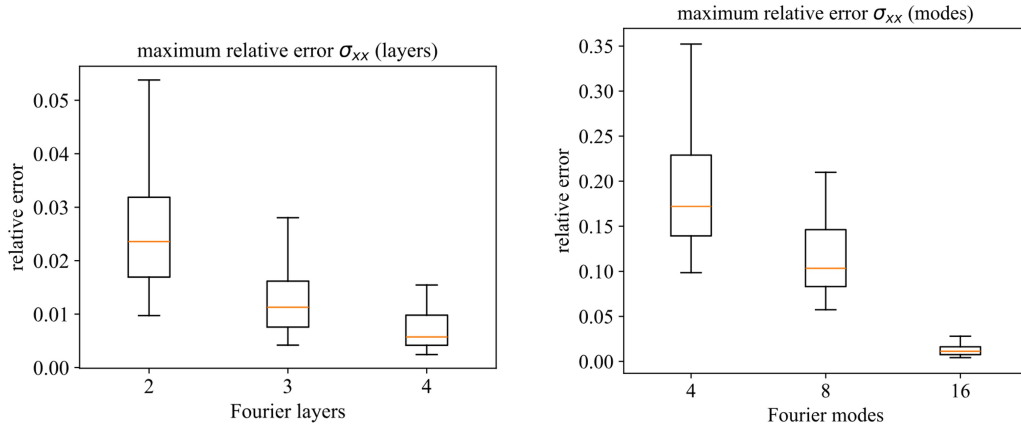


Figure S7: Hyperparameter studies for SPiFOL model. A study on the hyperparameters of the FNO model used for training the SPiFOL framework.

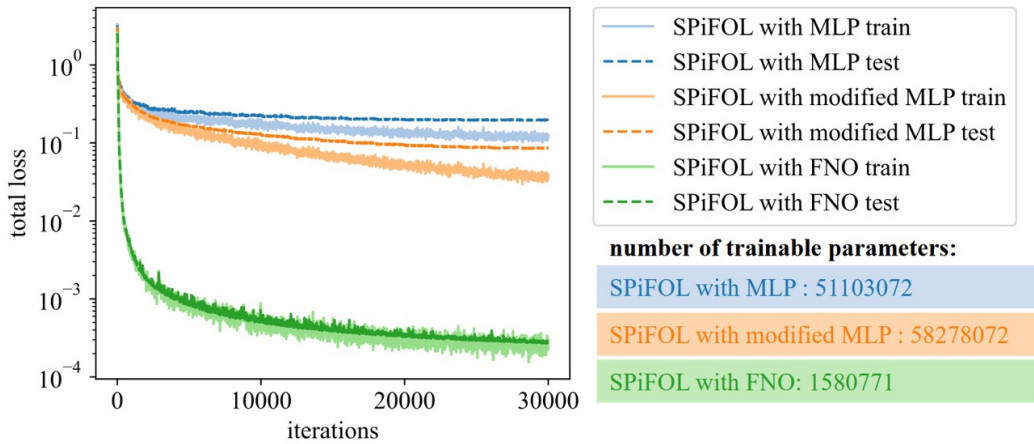


Figure S8: Training history for SPiFOL model. Loss decay and training history for the SPiFOL framework [4]

References

- [1] A. K. Boukellal, M. Rouby, and J.-M. Debierre. Tip dynamics for equiaxed al-cu dendrites in thin samples: Phase-field study of thermodynamic effects. *Comp. Mat. Sci.*, 186:110051, 2021. doi: 10.1016/j.commatsci.2020.110051.
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- [3] Openmmlab, 2024. Available: <https://github.com/open-mmlab>.
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