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Materials informatics: data-driven, materials design, and uncertainty quantification perspectives

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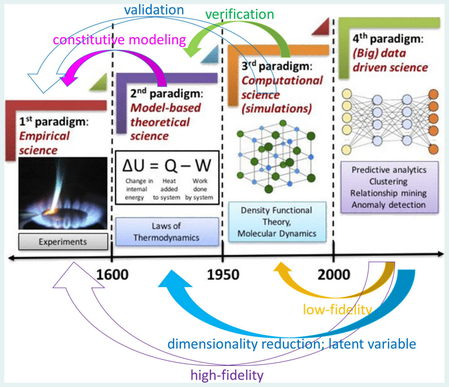
Motivation

Figure: Materials informatics as the fourth paradigm, adopted from Agrawal and Choudhary [1].



Uncertainty quantification of dendritic morphology using stochastic collation method [4]

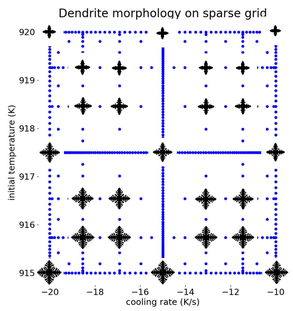


Figure: Representative dendritic morphology on SG as process parameters vary, i.e. cooling rate and initial temperature. The thermodynamic parameters are fixed at $\varepsilon^* = 0.35, \sigma_0^* = 0.24, M_\phi = 4 \cdot 10^{-9}$, respectively.

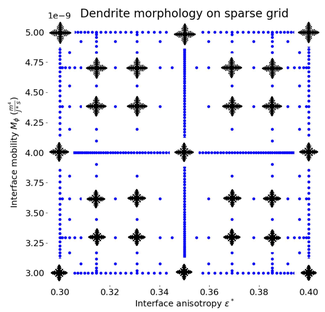


Figure: Dendritic morphology at different thermodynamic parameters on SG, where other parameters are fixed at $\frac{\partial T}{\partial t} = -15K/s$, $T_0 = 917.5$, and $\sigma_0^* = 0.24$.

- Clenshaw-Curtis points, $d = 5$, $q = 6$ sparse grid is used,
- 19,313 simulations are performed,
- 4 quantities of interests (QoIs) are post-processed using image-processing techniques.

High-fidelity data-driven microstructure reconstruction [3]

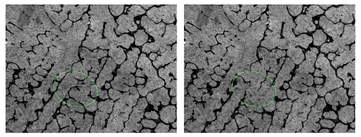


Figure: Orig. #35. Figure: Recon. #35.

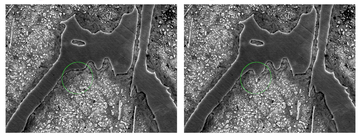


Figure: Orig. #1098. Figure: Recon. #1098.

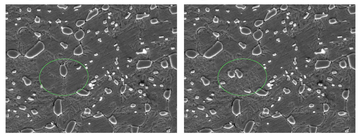


Figure: Orig. #1672. Figure: Recon. #1672.

Figure: Microstructure inpainting: Original and reconstructed microstructure on experimental micrographs from UltraHigh Carbon Steel micrograph DataBase.

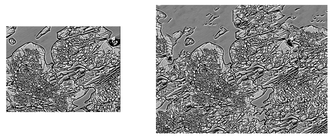


Figure: Orig. #1531. Figure: Recon. #1531.

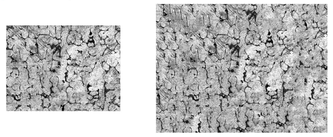


Figure: Orig. #1583. Figure: Recon. #1583.

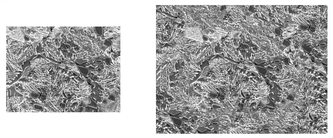


Figure: Orig. #1656. Figure: Recon. #1656.

Figure: Microstructure outpainting: Original and reconstructed microstructure on experimental micrographs from UltraHigh Carbon Steel micrograph DataBase.

- create synthetic high-fidelity microstructures,
- mitigate the data-hungry effect for deep learning applications with microstructures.

Bayesian optimization for learning processing parameters in kinetic Monte Carlo [2]

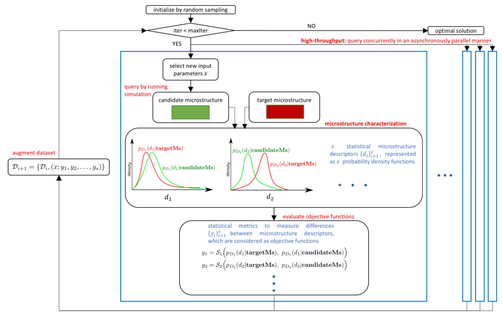


Figure: An overview perspective of the high-throughput microstructure calibration framework as a multi-objective optimization problem.

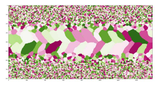


Figure: A rasterized ms. representation with dimension.

Figure: Grain 16166 in the ms.

Figure: Best fit ellipse (rotated 90° ccw).

Figure: Grain-based ms descriptors: Fitting ellipse process for a single grain in a microstructure.

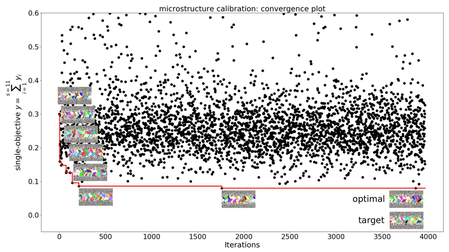


Figure: Convergence plot of the microstructure calibration framework. The objective is minimized as the optimization process advances.

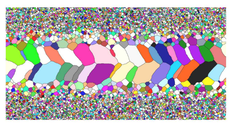


Figure: Optimal ms.

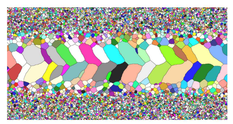


Figure: Target ms.

Figure: Comparison between optimal and target microstructures.

Physics-informed variational auto-encoder for microstructure

- capture the low-dimensional manifold of microstructure
- microstructure reconstruction applications
- data-driven process-microstructure-property linkage

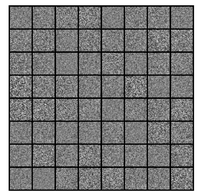


Figure: Epoch 1.

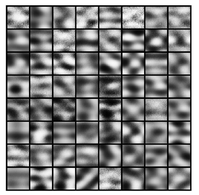


Figure: Epoch 81.

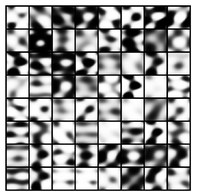


Figure: Epoch 6686.

Figure: Microstructure reconstruction with autoencoder for two-phase composite materials.

References

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