Challenges and Opportunities for Machine Learning Accelerated Materials Qualification for Brittle Particle Cold Spray

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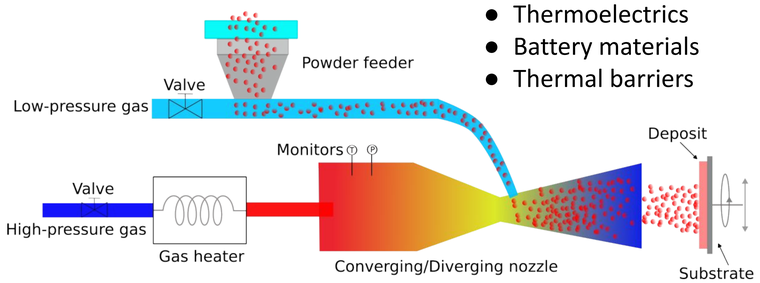
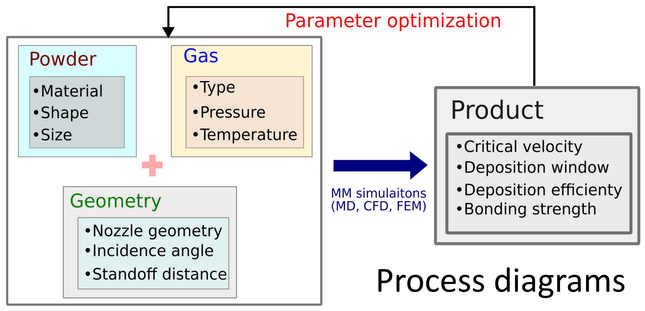
Introduction



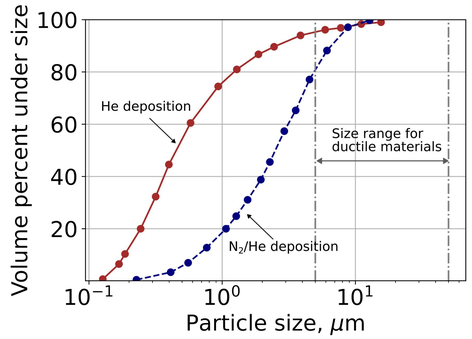
Brittle Particle Cold Spray

Potential applications
- Thermoelectrics
- Battery materials
- Thermal barriers

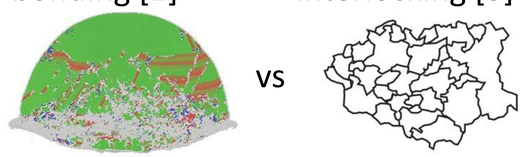


Process diagrams

Powder size distribution [1]

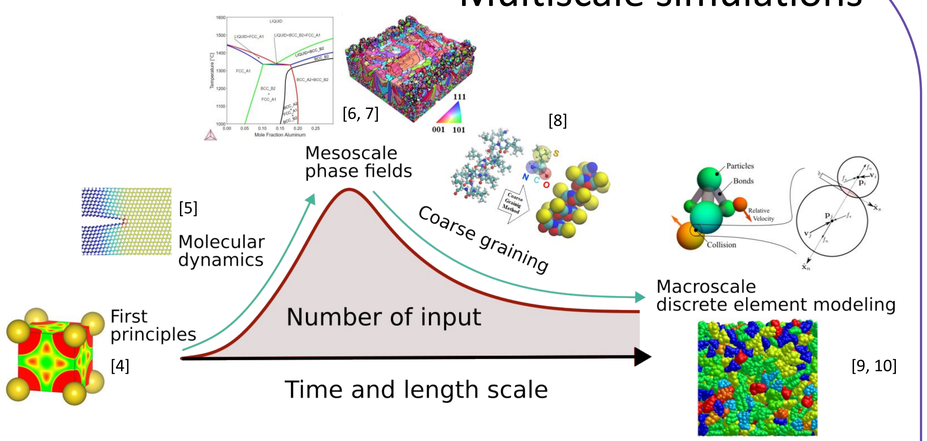


Metallurgical bonding [2] vs Mechanical interlocking [3]



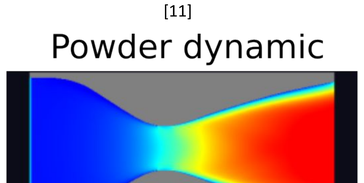
Objective: Accelerated materials qualification with machine learning

Multiscale simulations

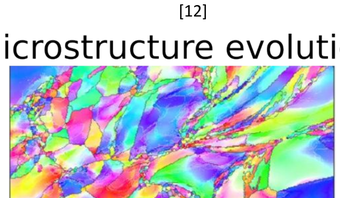


Multiphysics simulations

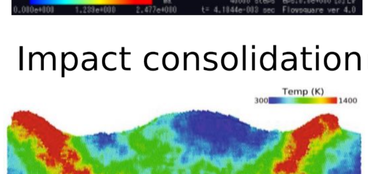
[11] Powder dynamic



[12] Microstructure evolution

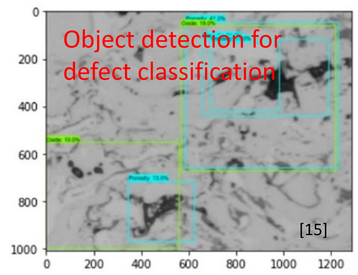


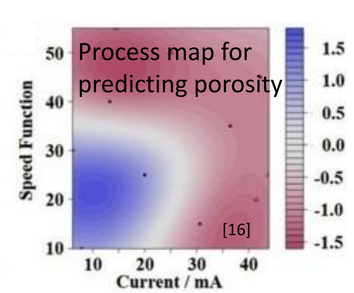
Impact consolidation [13]



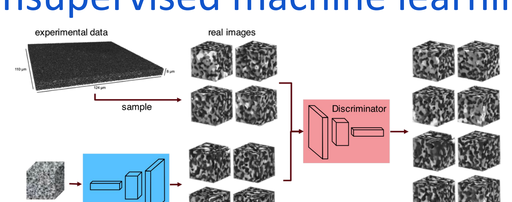
Residual stresses [14]

Supervised machine learning





Unsupervised machine learning



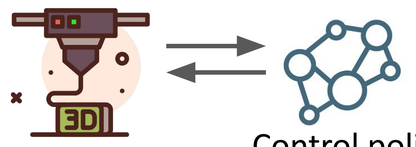
[17]

Challenges & Opportunities

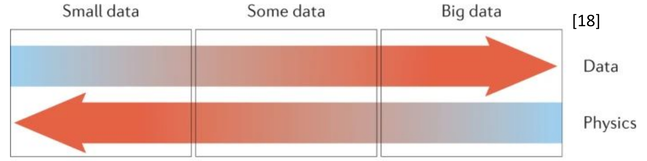
Data paucity, variability and noise	Data augmentation, Uncertainty estimate
Model complexity	Explainable AI
Physical understanding	Physics-informed models, Materials design

Future research directions

Digital twins

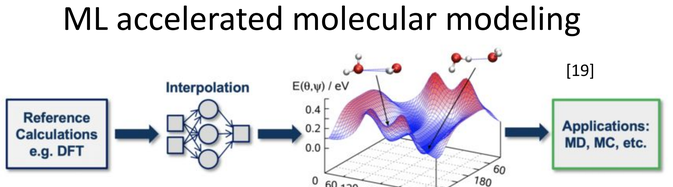


Physics-informed machine learning



[18]

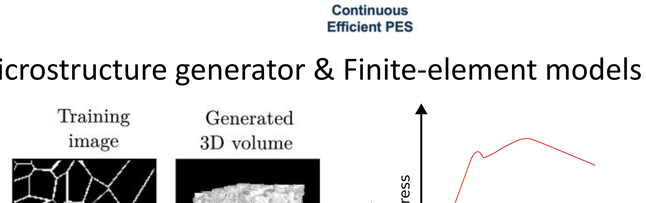
ML accelerated molecular modeling



[19]

Microstructure generator & Finite-element models

[20]



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[1] Figure courtesy to TTEC LLC in Virginia [2] Reddy et al, 2021. DOI: 10.1016/j.commatsci.2021.110363 [3] Bahrani and Kaiser, 2020. DOI: 10.1016/j.jrmge.2020.06.004 [4] Sun et al, 2023. DOI: 10.1073/pnas.2218405120 [5] https://libatoms.github.io/QUIP/Tutorials
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