

Materials Data and Models Across Scales

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Key challenge

- **Develop interatomic potentials (IAP) or crystal plasticity (CP) models “on-demand” with sufficient accuracy for a given application, with data from lower length scales**
- **Develop approaches to analyze the high-throughput, high-resolution data from additive manufacturing**

State of the art

- **Timely: Modeling frameworks and data are sufficiently developed, but still difficult to assess IAP accuracy based on DFT data or engineering scale CP models wrt microstructure variability**
- **Who else is doing this? NIST, GRANTA have large materials databases but mostly of properties not configurations**

New research direction

- **Develop ML alternatives to interatomic potentials or plasticity models (must incorporate physical constraints implicit in training data)**
- **Develop ML methods to analyze large datasets (meltpool, CT images) from high-throughput additive specimens**
- **Use ML approaches to develop Process-Structure-Property maps**

Potential scientific impact

- **New ML algorithms that incorporate physical constraints (e.g. rotational invariance, energy balance, flux, etc.)**
- **Advance ML methods to handle huge feature spaces of materials, phases, composition, configurations.**
- **Develop dimension reduction methods (PCA+tensor) to represent changing microstructures over time**