Are information sciences based approaches essential to allow predictive modeling of multiscale/multiphysics problems?

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Predictive materials modeling and design (in the presence of uncertainty) requires computing and controlling the induced variability of macroscopic properties.

- Multiscale sources of uncertainties
- Process & microstructure variability
- Location-specific microstructures
- Macroscopic models are phenomenological driven by (multiscale) data – obtained experimentally and from (more accurate) simulators at finer time- and length-scales.

Figures courtesy of Rolls Royce
Uncertainty Sources

**Macroscale uncertainties**
- Initial and boundary conditions (e.g. Die shape)
- Dual microstructures
- Process parameters:
  - Temperature
  - Strain rate
  - etc.

**Mesoscale uncertainties**
- Topology
- Two-phase features
- Orientation
- Model Parameters: CRSS, etc.

**Microscale uncertainties**
- Particle size/volume fraction
- Particle shape
- Dislocation configuration
- Parameters: APB energy, etc.
Predictive Materials Modeling and Design: An Information Theoretic Approach

- Quantifying input uncertainties
- Model reduction to account for the curse of dimensionality
- Solution of high-dimensional stochastic PDE and discrete based problems

- Stochastic coarse graining – uncertainty propagation across scales.
- Coarse scale problems are stochastic even if the microscale solvers are deterministic (uncertainty due to information loss)
- There are many mathematical & computational reasons why a stochastic/statistical framework is essential (predictability, complexity, ..)

Information theory, Bayesian inference/learning, and stochastic modeling are the only known tools with the potential of addressing such problems