Exploring position dependent property/microstructure relationships in polycrystal materials via probabilistic graphical model techniques

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We build a graphical model to represent the position dependent probabilistic relationship between the macroscopic properties and the underlying microstructures in polycrystal materials. The desired probabilistic graphical model can be viewed as a Bayesian mapping from microscale parameterizations to macroscale variables, which is similar to a regression from a high-dimensional input space to lower-dimensional output space. Based on the simulation data, we are aiming to create a robust and reliable probabilistic graphical model, in which we can quantitatively learn how the uncertainty propagates from one scale to another, and what is the correlation between the microscopic or macroscopic variables at different spatial points. Since the stochastic microstructure inputs are in high dimensional space, a model Reduction technique will be applied for the microscopic data before constructing the probabilistic graphical model. Once the graphical model has been built up, we can use it to predict the distribution of macroscopic properties for a new microstructure distribution.