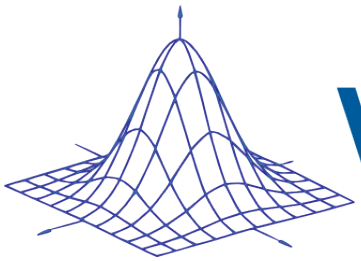

WCPM

Warwick Centre for Predictive Modelling Seminar Series

Uncertainty Quantification with Surrogate Models in Alloy Modeling

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Thu 8th Jan 4pm
LIB1, Lower Level, Main Library

Abstract: Surrogate models, e.g., the so-called cluster expansion, have been widely and successfully employed in alloy modeling to learn computationally expensive properties such as ab-initio energies, band gaps, and phase transition temperatures. Once learned, the surrogate is employed to quickly navigate the space of possible structures, e.g., to predict the largest band-gap structure, the lowest energy structure, or to map out the phase diagram of the alloy. Having an accurate and fast surrogate model is central to predictive success.

In this talk, we first demonstrate how information theoretic arguments can improve surrogates when used in thermodynamic modeling. The approach automatically shifts the attention of the surrogate model to thermodynamically relevant structures as temperature is changed. Second, a method is presented, which introduces rigorous uncertainty propagation in Materials Science. In particular, it is shown, within a fully Bayesian framework, how the uncertainty can be propagated from not knowing the best surrogate model and from not knowing the best data set, to the quantity of interest such as the alloy phase transition. We then discuss a novel method recently invented to improve the cluster expansion method when applied to arbitrary geometries of any shape on fixed underlying lattices. Finally, we discuss future directions which we believe will help to mature information theoretic approaches in Materials Science.

More info: http://www2.warwick.ac.uk/fac/sci/wcpm/seminars