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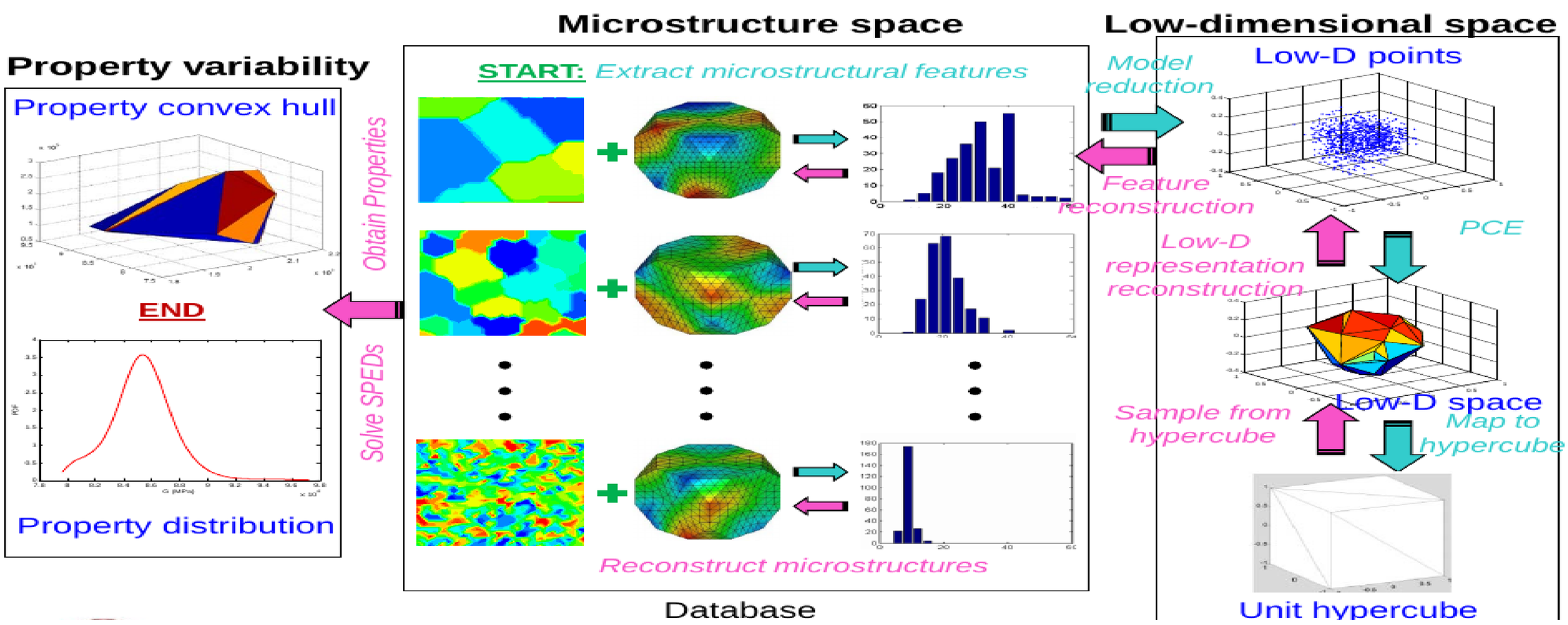
Seminar: An Information Theoretic Approach towards Predictive Materials Modeling

Prof. N. J. Zabaras, Cornell University

Time: Monday 7. April 2014 , 16:00

Place: Seminar room 2711 (Building 7, 2nd floor)



Abstract

Predictive modeling and design of materials gives rise to unique mathematical and computational challenges not present in other areas of physical sciences where modeling in the presence of uncertainties is important. Such challenges include but not limited to (i) Modeling of hierarchical **random heterogeneous material structures**; (ii) Propagating uncertainties in a quantifiable manner across spatial and temporal length scales (**stochastic coarse graining**); (iii) Addressing the curse of **stochastic dimensionality**; (iv) The limitations of phenomenology typical in most materials science models; (v) Modeling failure and **rare events** in random media; and many more.
We will briefly address these challenges in predictive modeling of heterogeneous media and discuss **data-driven models** of material structure, the curse of stochastic dimensionality in forward uncertainty propagation, stochastic coarse graining, development of inexpensive **surrogate stochastic models** and posing **multiscale problems in a graph theoretic framework**.
With synergistic developments in materials modeling, mathematics, statistics and scientific computing one maybe able to develop data-driven materials models that allow us to understand from where observable variabilities in properties arise, and how to control them to allow **accelerated materials design**.

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