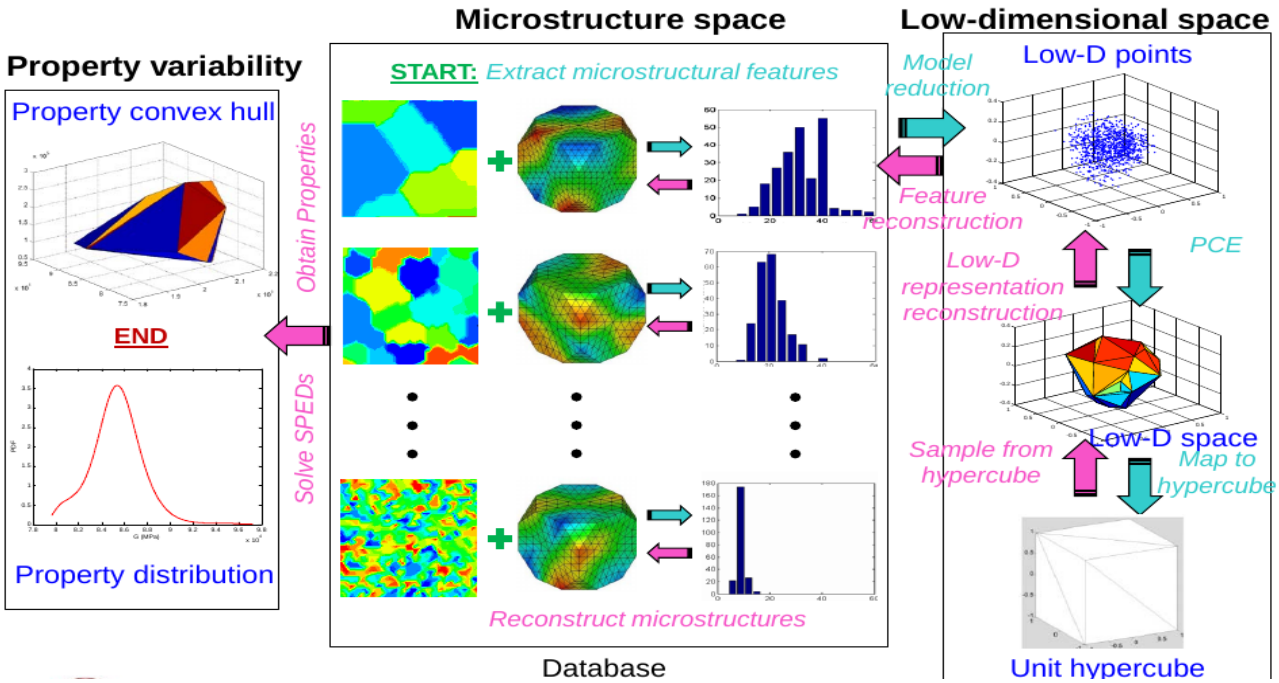
Ph.D Position on

Predicitive Materials Modeling



General Information

The following project is conducted in the context of the **Hans Fischer Senior Fellowship** (IAS – TUM) of **Prof. N. Zabaras** (Univesity of Warwick, http://zabaras.com/) and will be co-supervised by **Profs. Zabaras and Koutsourelakis** (Fachgebiet für Kontinuumsmechanik, MW, TUM).

Description

Uncertainty quantification (UQ) is arguably the fastest growing methodological paradigm in computer simulation of physical and engineering systems. Through data-driven methodologies, UQ is set to revolutionize modelling by augmenting bottom-up multiscale physically based models with data-driven approaches that improve predictive outcomes *and quantify the uncertainty in the predictions*. This paradigm will not only transform the use of modeling in science and engineering it will also facilitate the wider incorporation of predictive modelling across many industrial sectors.

The integration of uncertainty quantification with materials science is of paramount importance as material analysts always work with realizations of random microstructures, and materials and structures operate under random (or uncontrolled) operating and design conditions. The present project will pursue a set of fundamental problems in the interface of computational simulation and materials' engineering:

- ***Predictive Modelling of Multiscale/Multiphysics (Materials) Processes***: While modelling at individual scales has become routine, integration of scales remains an open issue both because of the disparity of length scales (time and space) and because of the lack of mathematical models with predictive ability that will allow us to link models across scales.
- **Emphasis on High Dimensionality:** Most applications in random materials lead to high stochastic dimensionality where existent UQ methods simply do not work. There are many opportunities to exploring ideas that from graph theory and probabilistic graphical models and variational methods.
- **Emphasis on Rare Events:** This is in many ways another unexplored area in the context of UQ. Existent approaches are simply not relevant e.g. in the context of materials where failure is not a single event describing the tails of a distribution at a given point. Failure and rare events have strong *dependence on the random microstructure environment (non-local effects).*
- **Integration of Computational Statistics & Machine Learning with Uncertainty Quantification:** Machine learning approaches provide an opportunity to address many multiscale problems as inference problems. Graphical models efficiently factorize the complex joint distribution of variables across and within scales, coarse graining can be posed (in a non-parametric fashion) as local inference problem, etc. These ideas may sound natural to the machine learning community but their application to multiscale scenarios requires innovative collaborative developments.
- **Data-Driven Design - Combinatorial discovery in materials:** We will seek to develop methodologies for rapidly mining materials databases in order to isolate and identify relevant information for the system's designer. This requires integration of (reduced-order) predictive materials models at different scales with statistical learning approaches. Such an approach will lead to rapid experimentation involving combinatorial processing and high-throughput screening, accelerated testing procedures at different scales.

Qualifications and how to Apply

- We are interested in **self-motivated, focused and hard-working** individuals with an ability for creative and innovative thinking.
- We are interested in applicants with strong academic backgrounds from all Engineering fields as well as Applied Mathematics, Applied Physics and Statistics. You can document your background by sending us by email an (unofficial) transcript of your academic record including courses/grades to **p.s.koutsourelakis@tum.de** by **September 1 2014**.
- Please include a **CV as well as a brief statement of your research experience** and any demonstrated programming skills.
- You are encouraged to contact Prof. Koutsourelakis (**p.s.koutsourelakis@tum.de)** if you have any questions on the re-quirements or the research activities of the group.