## Outwitting Gravity and Countering Uncertainty:

### Materials-by-Design

**Professor Nicholas Zabaras is using the resources of CTC to outwit gravity and the random nature of microstructures.**

In a project funded by NASA's office of Biological and Physical Research, Zabaras and his team in the Materials Process Design and Control (MPDC) Laboratory are controlling melt flow in crystal growth processes in order to reduce or eliminate the effects of gravity on crystal structures.

"We are not trying to get rid of gravity," said Zabaras. "We are getting rid of the effects of gravity. Can you do something to the flow of the liquid from which the crystal is grown to counter the complex effects of this flow on the growing crystal?"

The answer seems to be a resounding yes. The techniques Zabaras' team has developed use optimally selected, externally applied magnetic fields and magnetic field gradients along with controlled furnace conditions to finesse the effects of gravity on the obtained crystals, resulting in microgravity-like growth conditions.

Zabaras' work impacts the designs used for turbine blades and armor.

"Magnetic fields, the kind you find in a basic MRI machine, are one example of how you can design factory conditions to attack the effects of flow on crystal structure," said Zabaras. "Such techniques are applicable to various material systems including proteins. As a result, larger more perfect crystals can be formed, and perhaps entirely new materials, ones with the potential to help scientists make new medicines and predict diseases, will be created. Such controlled crystallization processes on earth may serve as an alternative to performing expensive lab experiments and crystal production in space."

The MPDC laboratory is also using parallel computation to develop a virtual environment for polycrystal materials-by-design. The project could have become an impossible mission. Sponsored by the U.S. Department of Defense (Air Force and Army), the National Science Foundation and industry, the project must deliver control at the micro level and insight into the evolution of the microstructure. Considering the random nature of the microstructure and the enormous size of the underlying optimization problems, this project provides significant challenges both mathematically and computationally.

"Our interests are not only to understand the effects of the microstructure on the properties of metallic materials, but also to design microstructures through processing leading to desirable properties for critical applications, such as the design of turbine blades and armor," Zabaras said. "Making sure that armor does not disintegrate when hit and that missiles detonate when and where they are expected to detonate provide enormous opportunities for the application of stochastic modeling and statistical learning."

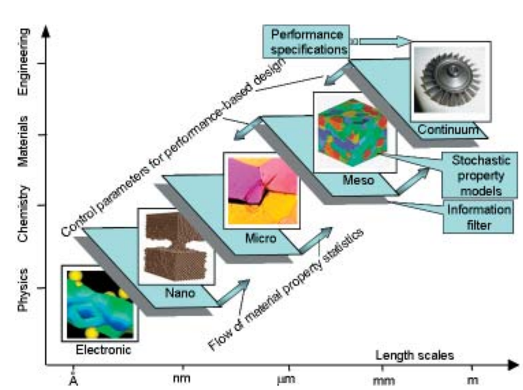
The team found opportunities in the challenge, though, and has demonstrated the importance of adapting and using techniques that have been successful in other fields. For example, the team is using mathematical model-reduction techniques to simplify complex physical models and image processing techniques to mathematically represent microstructure. These approaches are used in combination with hierarchical classification techniques that categorize microstructures and properties in classes based on common features.

"In understanding how statistical information flows from the microstructure to material properties, we are using an information-theoretic approach that illustrates information propagation and loss across length scales," added Zabaras.

Traditionally, this work has been done by averaging results when moving from one scale to another. There is an increasing demand to account for variability in material properties induced by microstructural heterogeneities and developing statistical multiscale methods that allow for uncertainty propagation across length scales.

"Parallel computation allows us to use innovative stochastic methods for such problems and treat uncertainty as an extra dimension in addition to space and time, thus capturing in one simulation its effect on modeling and design of complex material systems," Zabaras said.

A materials-by-design approach requires understanding the effects of structure on properties at various scales. Stochastic modeling and information-theory provide an important framework for understanding how information propagates from one length scale to another as well as the level of accuracy and sophistication needed at each scale to provide performance-related design (e.g. of a turbine blade) at the macro-scale.

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