

CAC and Nicholas Zabarar

Extreme Performance in the Presence of Uncertainties: a Virtual Materials-by-Design Framework

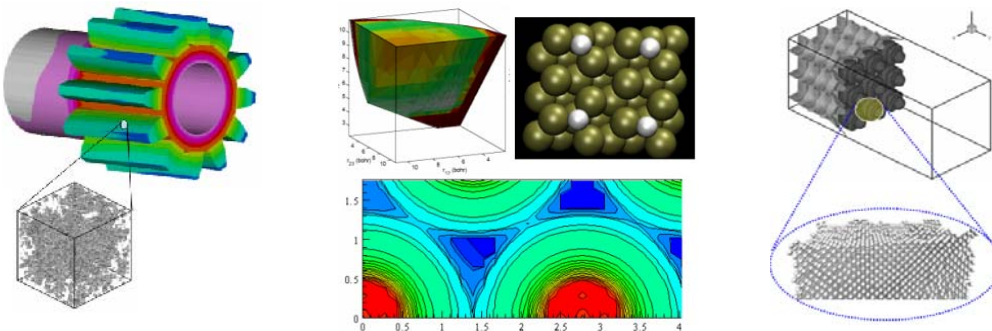
How do you develop a virtual environment for the design of new materials with extreme properties? How can materials be designed and tailored from the atoms up? How can extremities in operating conditions be included in the design matrix? How can property variations, fluctuations and uncertainties at the micro- and nano- scale be incorporated into robust design and control of critical components?

Finding the Answer

Nicholas Zabarar and Cornell's Materials Process Design and Control (MPDC) Laboratory are using CAC high-performance computing systems to accelerate the development of a virtual environment for materials-by-design. This virtual environment analyzes, quantifies and moderates the effect of uncertainties in operating conditions on the performance of critical polycrystalline based components (armor, ballistic coatings, heat shields, turbine blades) while concurrently providing a modular approach for designing novel materials using approaches from quantum chemistry.

Computational Materials-by-Design and Stochastic Analysis Enable Robust Component Design

The traditional approach to materials development and testing is time intensive and costly. Computational design is an emerging approach to the rapid development of new materials that have the specific characteristics and properties needed for products such a turbine blades and armor. Coupled with the ability to quantify the effects of uncertainties in operating conditions, this framework is a powerful computational technique for the robust design of critical, high-performance components.



Key ingredients: quantifying uncertainty + multiscale analysis + quantum chemistry

Improved Research

Research Metrics

- Design complex material systems using innovative stochastic methods and hyper-threading capabilities of the systems at CAC.
- Take into account the complete spatio-temporal effects (space, time and uncertainty): Model with parallel computing systems at CAC.

Research Challenge

Most metallic materials are aggregate composites of single crystals or polycrystals. “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,” Zabarás 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 at the macro-scale.

The challenge is providing 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 research provides significant challenges both mathematically and computationally.

Solution

The research team found opportunities in this challenge and has demonstrated the importance of adapting and using techniques that have been successful in other fields.

For example, the team uses 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 to 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 propagation and loss across length scales,” added Zabarás.

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.

CAC high-performance computing systems enable Zabarás and his research team to run more insightful simulations across multiple dimensions.

The Client

Nicholas J. Zabaras

- Professor, Sibley School of Mechanical and Aerospace Engineering, Cornell University
- Research focus on the computational design and control of materials processes, including deformation and solidification/crystal growth processes. Incorporating the effects of multiscale uncertainties in properties, structure and processes.
- Director, Materials Process Design and Control Laboratory
- Courses include “Atomistic Modeling of Materials”

The Collaborative Relationship

CAC provides parallel computing cluster access to Zabaras and his research colleagues to speed-up their applications and to help them address research problems not previously attempted.

“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 the modeling and design of complex material systems.”

Nicholas J. Zabaras

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