PURDUE UNIVERSITY | School of Nuclear Engineering

Nuclear Engineering Seminar

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Computational Material Science: Probing Material Behavior to Accelerate Nuclear Reactor Development

Abstract

Materials development is a slow process, with an average time span from discovering a new material to its deployment in the industry being about twenty years. The emerging field of material informatics, as the so-called “fourth paradigm,” holds promise to accelerate this process by integrating experiments, theory, and simulations in a data-driven approach using tools from artificial intelligence. The key aspect of this framework is the rapid development of process-structure-property-performance linkages by leveraging data science to enable application-specific design of materials in a top-down approach. This is even more crucial for nuclear applications, with the added constraint of performance under extreme environments and a high consequence on failure. In particular, material informatics is expected to play a key enabling role in the design of novel materials and the adoption of advanced manufacturing techniques like additive manufacturing in the nuclear industry. This talk covers a brief overview of computational material science and material informatics landscape for probing material behavior at different scales, followed by a few specific use cases from the speaker’s research.

Dr. Anant Raj is a post-doctoral researcher in the CYNICS group at the School of Nuclear Engineering, Purdue University. He received a Ph.D. and MS in Nuclear Engineering from North Carolina State University and a B.S in Mechanical engineering from Indian Institute of Technology Kanpur, India. He worked as a postdoc in North Carolina State University before joining Purdue and has over four years of experience working in the field of computational material science. His research particularly focuses on probing material behavior at different length and time scales for deducing process-structure-property relationships. His research interests include: materials under extreme environments, energy transport at nanoscale, phonons, advanced manufacturing, material informatics, artificial intelligence and machine learning. His most notable contribution has been in the development of computational tools for probing phonon transport in the framework of atomistic simulations.