Integrated Computational Materials Science and Engineering

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Currently, the design of components and parts for aerospace are limited to using decades-old available materials that have been through a lengthy and costly test and certification process. However, the current fiscal environment in which the DOD operates mandates an increased emphasis on affordability, flexibility, and rapid deployment of solutions, which demands desirable capabilities and properties beyond what these materials can provide.

Luckily, a wealth of research in material science and engineering has fostered a diverse class of candidates for the next generation of aerospace materials, including advanced composites, nanocomposites, and multifunctional materials. Unfortunately, these new materials face a formidable barrier to entry represented by an incomplete understanding of the materials, a lack of understanding of how to design for them, the lack of a readily available manufacturing infrastructure, and a lengthy and costly test and certification process.

At the same time, advanced modeling and simulation tools for conventional materials have become much more predictive, polished, and widely available, and there is growing hope that computational methods can enable rapid test and certification. However, software tools for design, simulation, certification, and manufacture of many of the most promising exotic new materials (sometimes inherently stochastic and/or multiscale) are not yet mature. ICMSE (Integrated Computational Materials Science and Engineering) is a vision led by AFRL to address this need.

The vision is to develop a new open, interoperable framework of software tools that can be used to design, certify, and manufacture novel materials and components. Properly designed, this would enable new designs (concurrent design of materials and components), allow cutting-edge manufacturing techniques to be exploited within the industry, speed test and certification, and eliminate barriers to introduction of materials to programs.

In order to succeed, such a software framework must enable trade-offs and optimization among three processes that are currently stovepiped for advanced materials: the materials selection, design, and manufacturing processes. Currently, a material is first selected based upon operational requirements. The design must then account for both the strengths and weaknesses of the particular material. The material is then manufactured; however, unexpected problems commonly arise, which may cause tests to fail. At this point, there is often no recourse but to start from scratch, resulting in time and money lost in significant redesign.

ICMSE would allow one to conceive of the part and simultaneously co-design the part and material, at all relevant scales (from the device scale, to the microscale, to even down to the quantum mechanical scale). We believe that this can be accomplished with today's tools, using a combination of multiscale modeling, informatics, and computational manufacturing capabilities.

This talk will center around Lockheed Martin's vision of the ICMSE framework, and what we view as outstanding critical needs for the vision to succeed.