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Materials Innovation Driven by Data and Knowledge Systems

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Current approaches for exploring materials and manufacturing (or processing) design spaces in pursuit of new/improved engineered structural materials continue to rely heavily on extensive experimentation, which typically demands inordinate investments in both time and effort. Although tremendous progress has been made in the development and validation of a range of simulation toolsets that capture the multiscale phenomena controlling material properties and performance characteristics of interest to advanced technologies, their systematic insertion into materials innovation efforts has encountered several hurdles. The most common of these are related to the lack of: (i) a generalized mathematical framework (applicable to a variety of materials classes and phenomena) that allows objective extraction and synergistic integration of the high-value materials knowledge (defined from the perspective of producing reliable process-structure-property [PSP] linkages) from all available datasets, including various multiscale experiments and simulations, while accounting for the inherent uncertainty associated with each dataset; (ii) formal approaches that identify objectively where to invest the next effort (e.g., a new experiment or simulation) for maximizing the likelihood of success (i.e., meeting or exceeding the designer-specified combinations of materials properties) at any step of the innovation effort; and (iii) experimental techniques specifically designed to provide the quality and quantity of information needed to calibrate the large number of material parameters present in most multiscale materials models. In this talk, Professor Kalidindi will describe ongoing efforts within his research group aimed at addressing these gaps that have hindered materials design progress.

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