Multiscale Modeling and Simulation of Materials: The Archetype-Genome Exemplar

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The unacceptably long time to discover new materials and incorporate them into applications is largely associated with the need to design new materials through a time consuming and repetitive cycle of testing and experimentation. The recently announced Materials Genome Initiative for Global Competitiveness outlines a program to drastically reduce the time to discover and insert new materials in applications. Central to this effort is a combination of advanced computational methods, the creation and sharing of big databases of materials properties, access to fast computers, and the development of algorithms that take advantage of the architecture of these machines. The construction of a genome from building blocks, termed archetypes, is the archetype-genome exemplar. All natural and synthetic systems critical to both mankind's infrastructure and the global ecosystem may be viewed in this physical representation. I will present the multiscale mathematical construction and computational implementation of new theories that contain new forms of balance laws and physically consistent constitutive relations that, by rethinking conventional multiscale mathematics, account for each piece of the genome assembly triplet: *archetypes, interactions, and their conformation*. Since archetypes and their interactions contain properties difficult to characterize with high fidelity, and since after mixing and processing these same archetypes conform into pseudo-random microstructures characterized by statistical descriptors, the material genome is governed by a statistical distribution that reflects these uncertainties propagating through the assembly process. The presence of uncertainty does not debar the quantitative prediction of material genomes; instead it forces predictions to be a genome's relevant statistical quantities such as its mean, correlations, and failure reliability. Applications to metallic material systems, polymer matrix composites, shape memory polymers design, and design of vibration isolation-energy harvesters will be given.

Vita: Dr. Wing Kam Liu, Walter P. Murphy Professor at Northwestern University, Founding Director of the NSF Summer Institute on Nano Mechanics and Materials, Founding Chair of the ASME NanoEngineering Council, Vice Chair of the US National Committee on Theoretical and Applied Mechanics within the National Academies, and Co-Founding Director of the Northwestern University Predictive Science and Engineering Design Program, received his B.S. from the University of Illinois at Chicago; his M.S. and Ph.D. both from Caltech. He is a world leader in multiscale simulation-based engineering and science and has applied a spectrum of atomistic, quantum, and continuum strategies towards the understanding and design of nano-materials, biological processes, and recently the use of organic and inorganic materials for drug delivery device, bio-sensing, and other diagnostic and therapeutic applications. The impact of his research contributions is attested by the large number of citations to his work (12,750 according to Institute for Scientific Information (ISI) with an H-factor of 57; 31,500 according to Google with an H-factor of 81). In 2001, he was cited by the ISI as "one of the most highly cited, influential researchers in Engineering, and an original member highly cited researchers database". Selected honors include the International Association of Computational Mechanics (IACM) Gauss-Newton Medal, the highest award given by IACM; the ASME Dedicated Service Award, the Robert Henry Thurston Lecture Award, the Gustus L. Larson Memorial Award, the Dedicated Service Award, the Pi Tau Sigma Gold Medal and the Melville Medal, (all from ASME); the John von Neumann Medal and the Computational Structural Mechanics Award from the US Association of Computational Mechanics (USACM), the highest honor given by USACM; and the IACM Computational Mechanics Award, and the Japanese Society of Mechanical Engineers. Liu chaired the ASME Applied Mechanics Division and is a past president of USACM. He is the editor of two International Journals and honorary editor of two journals and has been a consultant for more than 20 organizations. Liu has written three books; and he is a Fellow of ASME, ASCE, USACM, AAM, and IACM.