Recognition of Complex Biological/Nano Molecule Phenomena

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Abstract

The characterization and manipulation of complex biological systems have reached a stage where various levels of details must be resolved. This may range from the analysis of bulk blood flow inside the heart at the continuum level to the dynamics of a single focal adhesion contact at the molecular level. We briefly outline the immersed electrohydrodynamics finite element method (IEFEM) coupled with multiphysics features for solving a class of bio-nano-fluidics problems. We then apply the multiphysics of the composite electric field for the guided alignment of the carbon nanotube (CNT), viruses, and DNA. Preliminary results demonstrate that the proposed IEFEM provides an ideal modeling platform for the modeling of electric field guided assembly of nanowires and multi-physics biological systems, including arteries and cell-extra cellular matrix interaction. In collaboration with Professor Shu Liu of NU, we intend to enhance the retention of bone marrow-derived endothelial cell (EC)-like cells by molecular modulation in a matrix-based arterial reconstruction model for preventing thrombosis and intimal hyperplasia, develop an experimentation-computation-integrated model to analyze the adhesion properties of the EC-like cells and assess alterations in the adhesion properties in response to molecular modulation, and use the arterial reconstruction model as an example to demonstrate the significance of "molecular modulation of cell adhesion" for improving vascular function. Incorporating Kramers kinetic theory of chemical reactions into the IEFEM, the sub-cellular bonding and debonding of matrix ligands and integrin receptors between the substrate and the endothelial cell found in the inner lining of vessels can be modeled. The recognition of these molecular scale phenomena becomes essential and crucial to fundamentally analyze and characterize molecular activities that stimulate larger scale response. Such phenomena become vital in the emerging nanomedicine area of nanomaterial-enabled control and localization of drug delivery. It was recently found that nanodiamonds possess novel chemical, physical, and biological properties that can provide a transforming foundation for how drugs are delivered. It is believed the structure of the nanodiamond (ND) is crucial to the adsorption and desorption of drug molecules because it not only changes the self-assembly configuration but also alters the surface electrostatics. Understanding electronic structure of nanodiamonds may catalyze increased drug efficiency while minimizing patient side effects.

Vita: Dr. Wing Kam Liu 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 nano-materials for diagnostic and therapeutic applications. He was the first to develop concurrent multiscale methods for materials design. These methods have been used to design new alloys, composites, and various sensing and actuation devices. Selected honors include the Robert Henry Thurston Lecture Award, the Gustus L. Larson Memorial 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); and the Computational Mechanics Awards of the International Association of Computational Mechanics (IACM) and the Japanese Society of Mechanical Engineers. Liu chaired the ASME Applied Mechanics Division and is past president of USACM. He is listed by the Institute for Scientific Information as one of the most highly cited researchers in engineering. 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; the Meshfree Particle Methods book sets the standard in the field, the Finite element book becomes a classic, and the Nano Mechanics and Materials book received a very favorable review by Nanotoday (Nov, 2006).