Holistic Multi-scale Approaches for Nanotechnology Convergence Systems

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During the past decades, along with remarkable scientific and engineering achievements in many areas, the world has faced immense challenges. Increasing need for higher efficiency and reduction in system size motivates the investigation of novel nanoscale systems and materials. Various enhancements have been reported by tuning atomistic properties, chemical structures, and functionalities of advanced materials leading to eye-opening progress. The tremendous improvements in nanotechnology provide the necessary understanding of nanoscale physics to control and design the system properties, while at the same time focusing on the critical issue of integration with macroscopic system scales resulting in converging technology and phenomena at different time and length scales.

My research interest focuses on this challenging problem by introducing a novel holistic multi-scale integration in nanotechnology by hybridizing atomistic / molecular and mesoscale / continuum models, and developing unique methodologies for hierarchical integration of the complete system at different scales, and expanding to include multi-phenomena / physics (Fig.1). Information transfer from one scale to neighboring scales allows one to eventually predict macroscopic behavior or device scale functions from first principles in top-down / bottom-up / middle-out approaches. These approaches along with system optimization based on a clear understanding of nanoscale phenomena will lead to a novel multidisciplinary analysis paradigm.

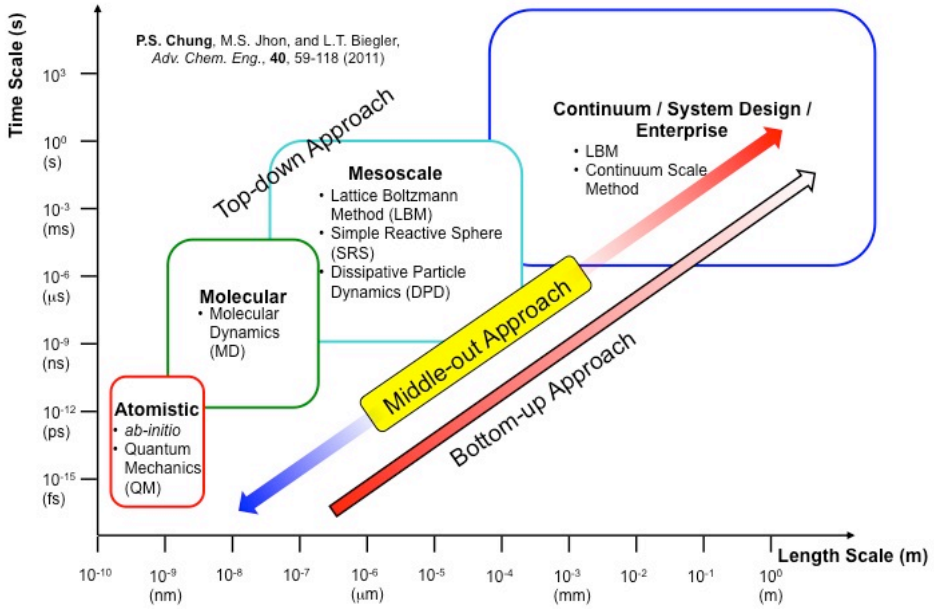


Fig.1. Hierarchy of multi-scale modelings and the integration methodology

In this poster session, I present case studies, which have been examined in the area of information technology and energy technology & sustainability for multi-scale modeling via a hierarchy of scale specific models coupled with optimization for the process system integration. Nano-tribology in the data storage system was chosen as a benchmark example utilizing atomistic / molecular simulations for the nanoscale film of functionalized oligomers / polymers with hybridization of novel graphene technologies and extended to mesoscale / continuum theories for the whole system integration [1,2]. In energy & sustainability area examples, we analyzed polymer electrolyte membrane fuel cell including membrane electrode assembly (polymer electrolyte membrane & catalyst layers) via atomistic / molecular simulations and transport phenomena in the gas diffusion layer via lattice Boltzmann method [3]. In addition, I will introduce and discuss the details of my future research topics and plan in this poster session.

Reference:

[1] P.S. Chung, S.H. Vemuri, S. Park, and M.S. Jhon, "Molecular rheological analysis on binary blends of perfluoropolyether lubricants," J. Appl. Phys., 115, 17B738 (2014).

[2] P.S. Chung, D.S. So, L.T. Biegler, and M.S. Jhon, "Nanotechnology convergence and modeling paradigm of sustainable energy system using polymer electrolyte membrane fuel cell as a benchmark example," J. Nanopart. Res., 14 (8), 853 (2012).

[3] P.S. Chung, R. Smith, S.H. Vemuri, Y.I. Jhon, K. Tak, I. Moon, L.T. Biegler, and M.S. Jhon "Multiscale/ multi-physical modeling in head/disk interface of magnetic data storage," J. Appl. Phys., 111 (7), 07B712 (2012).