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**“Multi-scale Modeling and Large-scale Simulations of Biotransports
in Nanothermo/Chemo-radiation Therapies**

Abstract

A thermo-therapeutic processing can be applied to either regional tumor (local hyperthermia) or the whole body (whole-body hyperthermia), depending on the tumor position, the cancer stage, and the health status of cancer patients. The major challenge in hyperthermia is to properly introduce a heat source for increasing tumor temperature during therapeutic process. Thermotherapy is often with chemo-radiation therapies. Such treatment brings not only promising but also challenges, since the tissue biotransport is very complex and the thermal-chemical dose profiles are coupled each other. Recently-developed nanothermotherapy brings a high promise to cancer and disease treatments. Induction of ferromagnetic or superparamagnetism (SPM) nanoparticles into a tumor region by injection or by blood-perfusion help terminate tumor cell lives. By applying an external electromagnetic field, nanoparticles help generate heat and reorient the direction to targeted tumor. The nanothermotherapy, on the other hand, yields challenges. It is urgent to develop a general model for simulate its clinical uses. Such demand requires an intensive study on the interactions of hyperthermia with tumor biological metabolism, its environments, the effects of angiogenesis and vasculature, blood perfusion, therapeutic gain of heat, etc.

The general model of biotransport (heat, mass, electromagnetism etc) must be developed based on multi-scales (nano-/micro-/macroscopic). The physical model must be full-field and simulation requires a petascale computing system. The thermal and mass conservations should be coupled. The thermo non-equilibrium which accounts for temperature differences should be considered. The thermal heat should be microscopically managed and monitored. The biotransport simulations use large-scale peta-scale high performance computing facility. The research results will be publicly useful in designing future Computer-Aided Planning (CAP) systems for clinical trials.

This presentation report our preliminary work on a simulator (multi-scale modeling, large-scale simulation, and clinical software) that contains a volume-averaged, generalized, multi-scale, multi-medium mathematical model of bio-electromagnetic (EM) - biotransport phenomena in a therapeutic process. The model accounts for nanoscale particulate motion, size and shape effects, microscopic cell and vasculatures, micro-fluid and heat transfer vessel perfusion, tumor tissue microstructure and morphology, energy and mass (dose and other biological compositions) conservation with proper physics-based constitutions, and interfacial heat/mass transfers for blood perfusion expressions and other micro-biological structures. The model equations are implemented numerically using lab's computing facility and NSF national petascale supercomputing facility at NCSA. Many geometric effects of nanoparticles, external alternate electromagnetic fields, nanoparticle materials, and biological properties of target tissue and vascular structures will be considered.

Bio

Dr. Jun Ni is an Associate Professor in Radiology, Biomedical Engineering, Mechanical & Industrial Engineering, and Adjunct Associate Professor in Computer Science. He has B.S from Harbin Engineering University in Naval Architecture, 1982; M.S. from Shanghai Jiao Tong University in Mechanical Engineering, 1984; and Ph.D. from UI, in Mechanical Engineering, 1991. He was a Post-doctor at Purdue University in Materials Processing, 1994. Since 1994, he was a senior consultant, research scientist, manager of scientific computing for University of Iowa research computing. He has been involved in many professional activities in different research fields. His current research (sponsored by NIH, NSF, Intel, and Microsoft and collaborated with Mayo, USC, Harvard, UTN, etc.) are high performance computing for medical imaging, and medical imaging or radiology informatics, nanotechnology/nanomedicine, and multi-scale model and simulations of transport phenomena in complex physical/biophysical and biomedical systems. Details of Dr. Jun Ni's research projects can be found at Lab Web site at www.uiowa.edu/mihpclub/ or Hawkeye Radiology Informatics project web site at www.uiowa.edu/hri/, two top "medical imaging informatics" indexed and lists on Google.