# Challenges in computational nanoscience

Risto Nieminen

Helsinki University of Technology, Finland

Nanosciences and their technological applications are among the major driving forces for tomorrow's society. The driving force for nanoscience and nanotechnology is to discover and manufacture materials and devices with new functionalities, not predicted by straightforward scaling from known macroscopic behavior. Mathematical modelling and large-scale computational simulation are important prerequisites for these efforts. They are needed to narrow down the enormous number of possibilities of assembling atoms and molecules to different structures and devices. In the nanoworld, the physical, chemical and biological properties of materials and structures are influenced by quantum phenomena, but require also proper treatment of statistical and stochastic processes. The challenges for the modelling and simulation efforts arise from (i) the requirement for quantitative accuracy to achieve predictive power; (ii) the computational complexity arising from the large number of interacting degrees of freedom and (iii) the necessity to bridge several orders of magnitude in both spatial and temporal domain in multi-scale modelling. Examples of current research topics in computational nanoscience will be discussed.