

The emerging field of multiscale simulation: Relation to cyber-infrastructure and educational needs

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Abstract

Multiscale simulation is emerging as a new scientific field in chemical sciences. The idea of multiscale modeling is straightforward: one computes information at a smaller (finer) scale and passes it to a model at a larger (coarser) scale by leaving out degrees of freedom as one moves from finer to coarser scales. The obvious goal of multiscale modeling is to predict macroscopic behavior of an engineering process from first principles (bottom-up approach). However, the emerging fields of nanotechnology and microtechnology impose new challenges and opportunities. For example, the ability to predict and control phenomena and nano-devices with resolution approaching molecular scale while manipulating macroscopic (engineering) scale variables can only be realized via multiscale simulation (top-down approach). In this talk recent developments in multiscale simulation will be reviewed. Examples of multiscale modeling will be presented from microchemical device design used for portable hydrogen production and for catalyst design used for catalytic combustion. Computational challenges and the symbiosis between multiscale modeling and cyber-infrastructure will be touched upon. Initial educational efforts on multiscale modeling will be discussed.