



ΙΔΡΥΜΑ ΤΕΧΝΟΛΟΓΙΑΣ ΚΑΙ ΕΡΕΥΝΑΣ

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ΘΕΜΑ: **The emerging field of multiscale simulation in the chemical and biological sciences**

ΤΟΠΟΣ: Αίθουσα Σεμιναρίων ΙΤΕ/ΕΙΧΗΜΥΘ

ΗΜΕΡΟΜΗΝΙΑ: Παρασκευή, 17 Ιουνίου 2005

ΩΡΑ: 12:00

ΠΕΡΙΛΗΨΗ

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 biotechnology 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. Developments from our work on coarse-grained Monte Carlo simulations and various types of hybrid multiscale simulation will be discussed. Examples of multiscale modeling will be presented from materials' self-organization for pattern formation leading to quantum dots and the epidermal growth factor receptor (EGFR) spatiotemporal dynamics on the surface of cell membranes.