



ΓΕΝΙΚΟ ΣΕΜΙΝΑΡΙΟ ΤΜΗΜΑΤΟΣ ΦΥΣΙΚΗΣ

PHYSICS COLLOQUIUM

Thursday, 10 April 2014

17:00 -18:00

3rd Floor Seminar Room

“Data driven, molecular dynamics for nanoscale flow simulations”

Prof. Petros Koumoutsakos

ETH, Switzerland

Abstract

Nanoscale flow phenomena are of fundamental importance to natural systems such as ion channels and to numerous technologies including energy efficient nanofiltration and molecular level drug delivery. We investigate the interaction of water with graphite and Carbon Nanotubes (CNTs) through large scale Molecular Dynamics (MD) simulations. Experimentally measured contact angles of nanoscale water droplets on graphitic surfaces are used to calibrate the parameters of the MD simulations. We employ these parameters to study water transport in micrometer thick, CNT membranes. Our simulations demonstrate transport enhancement rates that asymptote to 2 orders of magnitude over the continuum predictions. At the same time these rates are far below those that have been reported experimentally. I will discuss these discrepancies and suggest a Bayesian framework to consolidate experiments and MD simulations for the investigation of fluid mechanics at the nanoscale and their interface with continuum flow phenomena.