Abstract Submitted
for the DFD05 Meeting of
The American Physical Society

Multiscale Simulations of Carbon Nanotubes and Liquids PETROS KOUMOUTSAKOS, ETH Zurich — We present molecular dynamics and hybrid continuum/atomistic simulations of carbon nanotubes in liquid environments with an emphasis on aqueous solutions. We emphasize computational issues such as interaction potentials and coupling techniques and their influence on the simulated physics. We present results from simulations of water flows inside and outside doped and pure carbon nanotubes and discuss their implications for experimental studies.

Petros Koumoutsakos
ETH Zurich

Date submitted: 28 Jul 2005 Electronic form version 1.4