2012 Special Program in Applied Mathematics and Applied Mechanics

Reformulation of Maxwell's equations for molecular solutes

2012 - 05 - 09 (Wed.)
15:00 - 17:00
308, Mathematics Research Center Building (ori. New Math. Bldg.)

The dielectric polarization ***P*** surrounding the solute from Gauss's law is quite different with from molecular dynamics simulations using an explicit solvent model. For treating the problems such as protein folding, protein-protein/ligand interactions, or the effect of the external electric field to protein function, the electromagnetic equations were derived that (1) the solution of ***P*** behaves oscillation as distance to solute as from molecular dynamics simulations using an explicit solvent model, and (2) they can treat time-dependent electromagnetic interactions as Maxwell's equations do.