

数学与系统科学研究院

计算数学所学术报告

(系列讲座)

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(ICMSEC)

系列讲座题目:

Continuum modeling of
biomolecular systems (I, II, III)

报告题目: (讲座之二)

Continuum Modeling II:

II. PB electrostatics – Boundary
element method (continued)

报告时间: 2008年12月11日(周四)
下午3:00—4:00

报告地点: 科技综合楼三层311
计算数学所报告厅

Abstract:

The content of this part is: molecular surface definition and meshing; introduction of an efficient “node–patch” boundary element method; implementation of both the non–adaptive and adaptive fast multipole method into the BEM PB solver (AFMPB) to drastically speed up the solution; performance of our AFMPB solver; methods for electrostatic force and torque calculations in BEM framework as post–processing.

欢迎大家参加！