Applied Mathematics Seminar

INSCC 110, 3:30pm Monday

November 6, 2000

Issues and successes in molecular dynamics simulations of nucleic acid structure, dynamics and energetics

by

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Abstract

Thanks to advances in computer power and parallelization, methods for handling the long range electrostatic interactions and empirical force fields for bio-molecules, the last five years or so represent a renaissance in the simulation of nucleic acids. A brief review of some of the simulation highlights will be presented, with a focus on understanding the structure, dynamics, interactions and energetics of atomistic models of nucleic acids. Some methodological and representational issues that still need to be resolved will be discussed along with, hopefully, a discussion of potential areas that applied mathematicians may be able to lend some expertise.