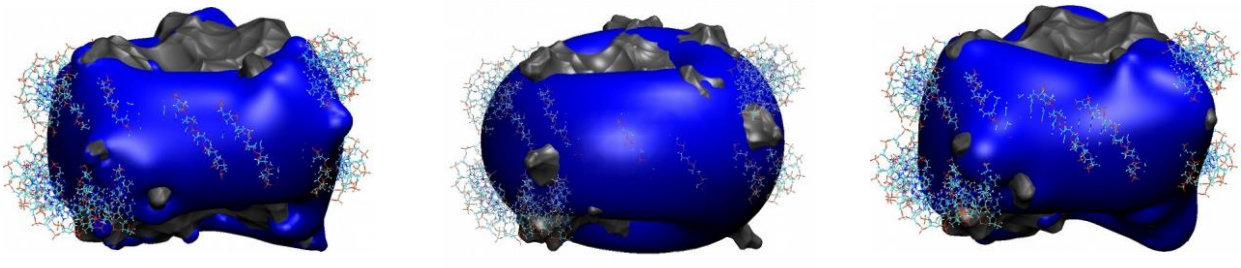
COLLOQUIUM



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Efficient Multipole Expansion Techniques

Abstract

Multipole expansions represent a standard technique in electrostatics. However, while very useful as a conceptual tool in analyzing asymptotic properties, the multipole expansions have rather limited applications in the ***practical*** numerical modeling of the electrostatic fields. The main limitations that prevent the application of the technique to many practical problems are the slow convergence and/or inapplicability of these expansions at short distances from the distribution of charges, and the dependence of these convergence properties on the center of expansion. These limitations are severely restrictive, for example, in the numerical modeling of the electrostatic filed in the immediate vicinity of the surface of large biological molecules. I will present the rankwise distributed multipole analysis (RWDMA), a method that improves the convergence and removes the ambiguity with respect to the center of expansion, and, if time permits, a partitioning algorithm which enables a multi-center multipole expansion that insures convergence outside any specified enclosing surface of the distribution of charge. I will illustrate the technique(s) with applications to the coarse-grained modeling of the field of some large biological molecules.

3:00-4:30 p.m., Friday, October 20th in McLane 162