

Abstract Submitted
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Efficient multipole expansion techniques for modeling the electrostatic field of large distributions of charge APOSTOL GRAMADA, PHILIP BOURNE, University of California San Diego — Despite being very useful as a conceptual tool, the multipole expansions have rather limited use in the *practical* numerical modeling of the electrostatic fields. What prevents their application to many practical problems are the slow convergence and/or inapplicability of these expansions at short distances from the distribution of charge, and the dependence of these convergence properties on the expansion center. These limitations are severely restrictive, for example, when modeling the electrostatic field of large biomolecules in the immediate vicinity of their surface. We present two techniques – the rank-wise distributed multipole analysis (RWDMA)¹ and a partitioning algorithm² – techniques that, together, overcome the above limitations, and illustrate them with applications to the coarse-grained modeling of the field of large biological molecules.

¹A. Gramada and P.E. Bourne, Phys. Rev. E 78, 066601 (2008)

²A. Gramada and P.E. Bourne, (submitted)

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