Treecode Algorithms for Long-Range Particle Interactions

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This presentation describes some recently developed treecode algorithms for computing long-range particle interactions in molecular dynamics simulations. The algorithms rely on Taylor approximation in Cartesian coordinates and use recurrence relations to compute the necessary Taylor coefficients. Adaptive techniques are employed to gain efficiency. Two algorithms are presented: (1) a particle-cluster treecode for the Ewald summation method in systems with periodic boundary conditions, and (2) a cluster-cluster treecode for the total potential energy in systems with vacuum boundary conditions. This is joint work with Zhong-Hui Duan (University of Akron).