A Direct Approach to Gravitation and Electrostatics

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A novel computational method to determine electrostatic interaction and gravitational potentials in three-dimensions (3D) by performing direct numerical integration is presented [1]. In the Direct Approach to Gravitation and Electrostatics (DAGE) method, the charge (mass) density and the potential are expanded in a finite-element basis set constructed as an outer product of one-dimensional (1D) Lagrange interpolation functions (LIF). The method does not involve any solutions of systems of linear equations, but the potential is obtained as a sum of differential contributions. Thus, no boundary conditions for the potential are needed. The method has been implemented and is shown to be accurate and computationally efficient. A parallel implementation of the algorithm shows that it is also well suited for parallel computers with a practically linear speed-up. The algorithm scales formally as $N^{4/3}$, where N denotes the grid size. However, by applying a divide-and-conquer strategy, the method can be made to scale linearly with the grid size rendering accurate calculations of the electrostatic potentials for very complex and extended molecular systems feasible.

[1]. D. Sundholm, J. Chem. Phys. (in press).

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