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Protein Electrostatics on a Desktop Using GPU Hardware and Multipole Algorithms

When studying the electrostatic interactions of molecules in solution, Poisson-Boltzmann solvers are a popular alternative to molecular dynamics. Among these solvers, the boundary element method (BEM) has become a competitive choice, compared to volume-based methods (finite difference, finite element). In BEM, the partial differential equation is formulated as a boundary integral problem for surface charge on the molecule-solvent interface, giving rise to a linear system. One disadvantage of BEM formulations is the generation of dense matrices, resulting in $O(N^2)$ complexity due to matrix-vector multiplications within iterative solvers. This precludes using more than a few thousand elements, which limits the accuracy that can be obtained with complex geometries, where finer discretizations are required. To obtain BEM solutions of large molecules, a fast algorithm for performing the dense matrix-vector multiplications is required. Treecodes or fast multipole methods have been used to reduce the complexity from $O(N^2)$ to $O(N \log N)$ or $O(N)$, respectively. Combining these fast algorithms with the latest GPU hardware, desktop calculations of protein electrostatics become practical even for large molecules.

Although we have previously developed high-performance tools for multipole-based algorithms on GPU clusters, in this work we focus on desktop solutions. We aim to provide a user-friendly environment for applying BEM in molecular electrostatics, using hardware and algorithmic acceleration. User-friendliness is provided by a Python interface to a GPU-enabled fast BEM (using PyCUDA). In this presentation, we will show benchmarking results of a BEM solver on GPU using an $O(N \log N)$ fast algorithm for the Yukawa kernel. The codes are being developed to be an open-source project.

We will show experimental results with physiologically relevant scales demonstrating that a full BEM calculation is indeed necessary. Even though the Yukawa kernel decays faster than, for example, the Laplace kernel, it does not decay fast enough to neglect far-field interactions (i.e., use a cutoff approach). Using a spherical molecule as a model, we find that in order to have an acceptable accuracy in the matrix-vector multiplication, at least half of the molecular surface needs to be considered in the matrix. Thus, a cutoff approach will still result in an $O(N^2)$ complexity, and neglecting the far field is not a feasible option when using large values of N.

In conclusion, the combination of fast algorithms and GPU architectures can enable a new level of computational research in biological applications, without the need to access large-scale systems and deal with complex code bases.