Exploring an Alternative Method to Compute Protein Electrostatics

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Protein electrostatics is the driving force behind molecular dynamics. The main equation governing these electrostatic forces is the Poisson Boltzmann equation for the potential. This project explores a novel approach to solving this equation. Instead of the standard finite difference or finite element methods we explore the use of the Boundary Element Method. The key to this approach is the implementation of the ACA algorithm to compress the matrix generated by the Boundary Element Method in hopes of generating an accurate result in a timely fashion. Another main component to the Boundary Element Method is the creation of a functional representation of the protein surface. Rather than using naïve spherical or cylindrical approach, we attempt to use a more precise spherical harmonics representation of the surface. The overall goal is an algorithm that can compute the potential in both a more accurate and a more timely fashion.