Department of Mathematics

University of Houston

Scientific Computing Seminar

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Computational Bioelectrostatics

Thursday, April 20, 2017
1:30 PM- 2:30 PM
Room 646 PGH

Abstract: Mathematical models of molecular solvation are crucial to the understanding of the physiological function and control of proteins, affecting the affinity and specificity with which biomolecules bind. Moreover, the solution of computational science problems is an interdisciplinary activity requiring mathematical, computational, and software expertise. I illustrate this process by considering the problem of protein solvation modeling from computational biophysics. Beginning with analysis of the relevant equations, I will explain the development of a new operator approximation for the boundary integral equations and prove bounds for the approximate solvation energy. By examining the special case of a spherical solute, we can make a finer grained analysis of the approximation, and are able to derive a much more accurate approximation. Finally, we demonstrate its excellent performance and scalability.