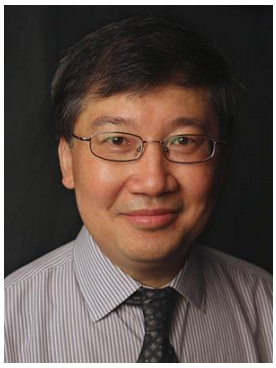
Joint Biomedical Engineering Seminar Series

MU ▪ MCW ▪ UWM

SEMINAR
Friday, March 2nd, 2018
12:00 – 1:00 pm
Kerrigan Auditorium
Medical College of Wisconsin



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"Recent advances in Development of Dielectric Continuum Models and Software Packages for Computing Electrostatic Salvation Free Energy of Biomolecules"

Calculation of electrostatic salvation free energy for a protein (or other biomolecules) in an ionic solvent is a fundamental task in structural biology, biochemistry, biophysics, and bioengineering. The Poisson-Boltzmann equation (PBE) is one commonly used dielectric continuum model for such a task. It has been applied to protein study, rational drug design, and many other bioengineering applications. To reflect polarization correlation among water molecules and ionic size effects, we recently developed new variants of PBE, called the size modified PBE (SMPBE), nonlocal modified PBE (NMPBE), and nonlocal Poisson-Fermi (NPF) models, along with the related numerical solvers and software packages. In this talk, I will report these recent advances. In particular, I will introduce our new SMPBS (Size Modified Poisson-Boltzmann Solvers) web server (smpbs.math.uwm.edu), which was published on the Journal of Computational Chemistry in the last year. SMPBS will be demonstrated as a useful tool for predicting the electrostatic solvation free energy of a protein in a symmetric 1;1 ionic solvent. Our research projects were partially supported by the National Science Foundation, USA, through grants DMS-0921004 and DMS-1226259.

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Medical College of Wisconsin is located at 1101 N. 87th St., Milwaukee, WI 53226. Parking is available across the street in visitor parking. Refreshments will be served.