Publications

Benzhuo Lu

Invited review:

1. B. Z. Lu, Y. C. Zhou, Michael J. Holst, and J. A. McCammon. Recent progress in numerical solution of the Poisson-Boltzmann equation for biophysical applications. *Commun. Comput. Phys.*, preprint, 2007.

Journal paper:

[1] B. Z. Lu and et al. Molecular boundary-free continuum model of electrodiffusion for biomolecular systems. preprint.

[2] Y. C. Zhou, B. Z. Lu, Gary A. Huber, Michael J. Holst, and J. A. McCammon. Continuum simulations of acetylcholine consumption by acetylcholinesterase - a Poisson-Nernst-Planck approach. accepted.

[3] B. Z. Lu, Y. C. Zhou, Gary A. Huber, Stephen D. Bond, Michael J. Holst, and J. Andrew McCammon. Electrodiffusion: A continuum modeling framework for biomolecular systems with realistic spatiotemporal resolution. *J. Chem. Phys.*, 127(13):135102, 2007.

[4] B. Z. Lu, X. L. Cheng, and J. A. McCammon. "New-Version-Fast-Multipole Method" Accelerated Electrostatic Calculations in Biomolecular Systems. *J. Comput. Phys.*, 226(2):1348–1366, 2007.

[5] B. Z. Lu and J. A. McCammon. Improved boundary element methods for Poisson-Boltzmann electrostatic potential and force calculations. *J. Chem. Theory. Comput.*, 3(3):1134–1142, 2007.

[6] B. Z. Lu, X. L. Cheng, J. F. Huang, and J. A. McCammon. Order N algorithm for computation of electrostatic interactions in biomolecular systems. *Proc. Natl. Acad. Sci. U. S. A.*, 103(51):19314–19319, 2006.

[7] T. J. Hou, K. Chen, W. McLaughlin, B. Z. Lu, and W. Wang. Computational analysis and prediction of the Binding Motif and Protein Interacting Partners of the Abl SH3 domain. *PLoS Computational Biology*, 2(1):e1, 2006.

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[12] B. Z. Lu, X. L. Cheng, T. J. Hou, and J. A. McCammon. Calculation of the Maxwell stress tensor and the Poisson-Boltzmann force on a solvated molecular surface using hypersingular boundary integrals. *J. Chem. Phys.*, 123(8):084904, 2005.

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[14] B. Z. Lu and C. F. Wong. Direct calculation of entropy loss due to reduced translational and rotational motions upon molecular binding. *Biopolymers*, 79:277–285, 2005.

[15] Y. H. Yu, B. Z. Lu*, J. G. Han, and P. F. Zhang. Scoring the protein-protein docked structures based on the balance and tightness of binding. *J. Comput. Aided Mol. Des*, 18(4):251–260, 2004.

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ORAL PRESENTATIONS ON CONFERENCES

"Finite element Poisson-Nernst-Planck approach for electrodiffusion and reaction processes in biomolecular systems" (to be attending) on January 4-8, 2008 at the Pacific Symposium on Biocomputing, session "Multiscale Modeling and Simulation: from Molecules to Cells to Organisms", The Big Island of Hawaii, January 4-8, 2008.

"Electrostatics, density distribution, and diffusion - A continuum modeling frame with realistic spatiotemporal resolution" on March 7, 2007 at the Biophysical Society 51st Annual Meeting. Baltimore, Maryland, MD, March 3-7, 2007.

"Accelerating computations to order N for electrostatic interactions of biomolecular systems" on Sep. 11, 2006 at the 232nd ACS National Meeting, San Francisco, CA, September 10-14, 2006.

"Molecular Simulations of Protein Kinase A: Release of ADP from the catalytic subunit of PKA: A MD simulation study" on July 12, 2005 at ICAM Frontiers of Science Symposium: Signal Transduction and Protein Phosphorylation, UC San Diego, CA.

"A new minimization method for real protein folding prediction," presented on May. 30 at the Seventh Symposium on Life Science at Home and Abroad, the Academy of military medical sciences, Beijing, China.

"Dynamics simulation for protein-protein interaction" at Proceedings of Chinese Biomedical Engineering 2001 (CBME), Wuhan, China.

POSTERS

"A calculation method of Poisson-Boltzmann forces between solvated macromolecules" on Biophysical Society 50th Annual Meeting, February 18-22, 2006, Salt Lake city, Utah.

"Rate constant calculation of ligand binding with solvation force determined by boundary elementary method" on Mar. 13, 2005 at the 229th American Chemical Society National Meeting & Exposition, San Diego, CA

"Effect of E230Q to the synergistic binding of ATP and PKI to the catalytic subunit of PKA" on July 30, 2005 at 19th Annual Symposium of The Protein Society: The Integration of the Cellular Protein Machinery: Complexes to Networks, Boston, Massachusetts.