Kei Moritsugu

Computational Science Research Program, RIKEN
2-1 Hirosawa, Wako, 351-0198
E-mail: moritsuguk@riken.jp

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April 1994	B.S., at Faculty of Science, Kyoto University
April 1998	M.S., at Graduate School of Science, Kyoto University
April 2000	Ph.D., at Graduate School of Science, Kyoto University
April 2003	Postdoctoral fellow at Graduate School of Integrated Science, Yokohama City University
September 2003	Postdoctoral fellow at Interdisciplinary Center for Scientific Computing (IWR), University of Heidelberg
April 2004	Research Fellow of the Japan Society for the Promotion of Science (JSPS)
March 2007	Postdoctoral fellow at the Center for Molecular Biophysics, Oak Ridge National Laboratory
November 2007	Research Scientist at Computational Science Research Program, RIKEN

Coarse graining methodology for the multiscale simulation of complex biological systems

Computer simulation holds the promise of revealing the mechanisms of biological processes in their ultimate detail. Although atomistic molecular dynamics (MD) simulation using molecular mechanics potential functions has provided crucial insight into many aspects of chemical and biophysical systems, the characteristic times of biologically relevant processes remain out of reach. Here, a coarse graining methodology is presented for extending the size and timescale of the systems to be simulated. The multiscale development involves, (1) coarse graining via implicit solvent using Langevin equation, and (2) that of atomistic potential function onto residue-scale force field via our REACH method.

The two methods follow the same scheme in that mapping on the coarse-grained model is performed using all-atom MD simulation based on the all-atom potential energy function. In (1), the velocity autocorrelation function for each normal mode calculated from the atomistic MD was fitted to that from the Langevin equation, leading to a friction coefficient. The atomistic frictions were then derived from the solution and vacuum MD, allowing the solvent contribution to the friction to be examined. Langevin dynamics MD was performed to examine whether the implicit solvent MD including the derived atom-dependent frictions can reproduce the solution MD result. In (2), the residue-scale elastic network force constants were calculated from the atomistic MD for three proteins to show the transferability of the REACH method. The REACH force field was extended by combining with a double-well potential, allowing structural changes of the ligand-unbound adenylate kinase to be represented via residue-scale coarse-grained MD.