Monthly informal seminar series on

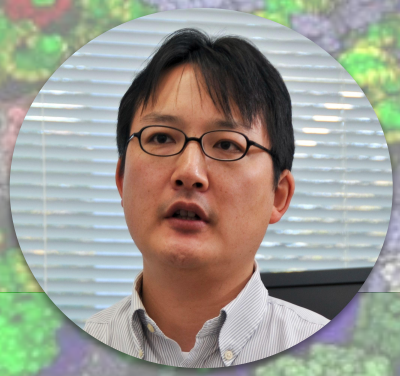
Integrative Modelling in Biophysics

presented by

Molecular Biophysics Unit, IISc

Multi-scale molecular dynamics simulations of biomolecules in cellular environments

Proteins, nucleic acids, and other biomolecules are all working in the cells. The environments are highly heterogeneous and crowded with so many biomolecules. How biomolecules can function properly in such cellular crowded environments is still a great mystery. To answer this question computationally, high-performance MD simulations and efficient sampling algorithms are both necessary together with accurate potential energy functions (force fields). In our group, we have developed high-performance MD software, GENESIS, (https://www.r-ccs.riken.jp/labs/cbrt/) and allowed to simulate large biological systems using supercomputers like K or Fugaku in Japan. We have also developed the generalized-ensemble algorithms, for instance, replica-exchange molecular dynamics (REMD) method, generalized replica-exchange with solute tempering (REST), and so on. In this talk, we will discuss the development of MD software and enhanced sampling methods implemented in GENESIS. They are useful to investigate slow biological processes, such as protein-ligand binding and protein conformational changes in various cellular environments. We will introduce some of our recent simulations using GENESIS on K or Fugaku supercomputers.



Prof. Yuji Sugita

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Yuji Sugita is a chief scientist in Theoretical Molecular Science Laboratory at RIKEN Cluster for Pioneering Research in Japan. He graduated from Department of Chemistry, Graduate School of Kyoto University (1998) and received his Ph.D degree (1998) (supervised by Prof. Nobuhiro Go). After a short postdoctoral fellow experience in RIKEN, he moved to Institute for Molecular Science (IMS) as a research associate (1998) and wrote the first paper of replica-exchange molecular dynamics (REMD) simulation together with Prof. Yuko Okamoto. In 2002, he moved to the Institute of Molecular and Cellular Biosciences, the University of Tokyo and started MD simulations of Calcium Ion Pump with Prof. Chikashi Toyoshima. From 2007, he has worked in RIKEN as a PI (associate chief scientist (2007-2012) and chief scientist (2012-present)). His current research interest is the development of MD software GENESIS and biomolecular simulations in cellular environments.

Date: 11-Jan-2022 (Tuesday)
Time: 17:30 hours (IST)

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