第２回レア･イベントの理論科学ワークショップのお知らせ

Transition Path Sampling などのレア･イベントを扱う統計力学手法開発で著名な Peter G. Bolhuis 教授が ICMS2013 で来日される機に、「レア･イベントの理論科学」に関するワークショップを企画しました。また、計算科学的な手法開発を精力的に進められている志賀基之博士(原子力機構)、森下徹也博士(産総研)をお招きして、最新の研究成果についてお話しいただく予定です。ご興味の皆様のご来聴をお待ちしております。なお、講演は英語で行われます。

日時：平成 25 年 11 月 21 日(木)　13:30-17:30
場所：産業技術総合研究所　関西センター(大阪府池田市)
　　産学官研究交流棟 3F　交流コーナー(3012 室)
　　(http://unit.aist.go.jp/kansai/access.html)
参加費：無料

プログラム：

13:30-14:45　“Enhanced simulation of protein folding and self-assembly”
　　Prof. Peter Bolhuis (Univ. Amsterdam)
14:45-15:00　Coffee Break
15:00-16:00　“Challenges toward ab initio molecular simulations of rare events”
　　Dr. Motoyuki Shiga (JAEA)
16:00-17:00　“Logarithmic mean-force dynamics for free-energy construction
　　without postprocessing”
　　Dr. Tetsuya Morishita (AIST)
17:00-17:30　Free Discussion

＊なお 18:00-21:00 池田駅周辺で懇親会(実費)を予定しております。

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Enhanced simulation of protein folding and self-assembly

Peter G. Bolhuis (Univ. Amsterdam)

All-atom molecular dynamics (MD) simulations of folding, conformational changes and self-assembly of proteins remain a great challenge because of the long time scales involved. These long times are due to high free energy barriers between metastable states. One approach is to invoke rare event methods such as Replica Exchange MD and Transition Path Sampling (TPS) to overcome these barriers. Another is to employ coarse grained models. I will present recently developed improved path sampling methods, and discuss application of these methods to protein folding. In addition, I will discuss protein self-assembly into fibrils using a coarse-grained approach in combination with replica exchange. In each case we obtain significant novel insight on the mechanism and the kinetics of protein folding and assembly.

Challenges toward ab initio molecular simulations of rare events

Motoyuki Shiga (JAEA)

In this talk, I will give a couple of recent topics on challenges toward ab initio simulations of rare events [1-3]. The first part is about the reaction path calculation of quantum systems. A generalization of the intrinsic reaction coordinate (IRC) is suggested for quantum many-body systems described in terms of the mass-weighted ring polymer centroids in the imaginary-time path integral theory, the "centroid IRC" [1]. This is applied to ammonia molecule and deprotonated ammonia dimer as well as their deuterated species to study the importance of nuclear quantum effects in the intramolecular and intermolecular proton transfer reactions, using ab initio path integral simulation combined with the string method. The second part is about the efficient sampling for QM/MM simulations of diffusive systems. A bias potential is suggested such that it separates the particles in the QM and MM regions while preserving the correct statistical distribution of the canonical ensemble [2]. The method is applied to ab initio QM/MM simulations of aqueous alkali ions. It is shown that the multiple-time-scale technique helps overcome the sampling bottleneck for such QM/MM simulations [3]. I will also mention the future challenges of path sampling simulation based on Onsager-Machlup action [4,5].

[1] M. Shiga and H. Fujisaki, J. Chem. Phys. 136, 184103 (2012).
[2] M. Shiga and M. Masia, J. Chem. Phys. 139, 044120 (2013).
[3] M. Shiga and M. Masia, J. Chem. Phys. 139, 144103 (2013).
[4] H. Fujisaki, M. Shiga, A. Kidera, J. Chem. Phys. 132, 134101 (2010).
[5] H. Fujisaki, M. Shiga, K. Moritsugu, A. Kidera, J. Chem. Phys. 139, 054117 (2013).

Logarithmic mean-force dynamics for free-energy construction without postprocessing

Tetsuya Morishita (AIST)

In this talk, I will introduce a new method for free-energy calculation based on mean-force dynamics (a fictitious dynamics on a potential of mean-force). The new method, logarithmic mean-force dynamics (LogMFD) [1], utilizes a logarithmic form of free-energy to enhance crossing barriers on a free-energy landscape, which results in efficient sampling of rare events. Invoking a conserved quantity in mean-force dynamics, the free-energy can be estimated on-the-fly without postprocessing. The new method is benchmarked against conventional methods and its high efficiency is demonstrated in the free-energy calculation for a coarse-grained model of protein-G [2].

[1] T. Morishita et al., Phys. Rev. E 85, 066702 (2012); J. Comp. Chem. 34, 1375 (2013).
[2] M. Isobe, H. Shimizu, and Y. Hiwatari, J. Phys. Soc. Jpn, 70, 1233 (2001).