RICC Usage Report for Fiscal Year 2010

Project Title:
MD Simulations on Si-Clathrates and Biomolecules with DL_POLY/MDGRAPE-3 and AMBER

Name:
Kholmirzo Kholmurodov
Toshikazu Ebisuzaki
Toshiaki Iitaka

Affiliation: Computational Astrophysics Laboratory
Advanced Science Institute  Wako Institute

1. Since 1997, our research teams from JINR (Principal: Dr. Kholmirzo KHOLMURODOV) and RIKEN (Principal: Dr. Toshikazu EBISUZAKI) have been performing long-term and very productive joint research on molecular dynamics simulation of material science and biological problems. We have published several joint papers in international and domestic scientific journals; presented joint papers at international meetings and conferences. We have organized and successfully performed several International Workshops "Molecular Simulation Studied in Material and Biological Sciences" (MSSMBS) in 2004, 2006, 2008, and 2010 on methodological and application aspects of the art of molecular dynamics simulation. We have experience of joint MD research on different kinds of computers of parallel or vector architectures. During many years, we have been developing simulation techniques, methods, and computer codes under specialized computing architectures, like MDGRAPE-2 and 3 (Tflop and Pflop calculation speed for large biological systems).


4. The Use of the MD Simulation Method is One of the Effective Approach for Discovering New Phenomena and Structural Properties of the Nano-Bio-System.

5. April 2011 – April 2012.

6. We continue MD simulations for the several system sizes on the objects as outlined in the project. The obtained simulation data indicate on the possible pathways of the dynamical changes and structural behavior.
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**Fiscal Year 2010 List of Publications Resulting from the Use of RICC**

**[Publication]**


**[Proceedings, etc.]**


**[Oral presentation at an international symposium]**


**[Others]**