Project Title: MD Simulations on Material Science Models and Biomolecules

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1. Background and purpose of the project, relationship of the project with other projects
We have performed molecular dynamics (MD) simulations for materials science and biological subjects. We do have experiences 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). We published joint papers in international and domestic scientific journals; presented joint studies at international meetings and conferences. We have organized and successfully performed several Japan-Russia International Workshops "Molecular Simulation Studied in Material and Biological Sciences" (MSSMBS) in 2004-2012, The MSSMBS workshops are devoted to methodological and application aspects of the art of molecular dynamics simulation.

2. Specific usage status of the system and calculation method
General Use Status of the RICC System.
Molecular Dynamics (MD) Calculation Method.

3. Result
New Structural Data of Nano- and Biomolecules.

4. Conclusion
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. Schedule and prospect for the future
April 2012 – April 2013.

6. If you wish to extend your account, provide usage situation (how far you have achieved, what calculation you have completed and what is yet to be done) and what you will do specifically in the next usage term.
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.
RICC Usage Report for Fiscal Year 2012

Fiscal Year 2012 List of Publications Resulting from the Use of RICC

[Publication]


12. Kholmirzo KHOLOMURODOV, "Molecular Modeling in Biological (Protein) and Material Research", Scientific Seminar of Thermal Physics Laboratory, Department of Engineering Physics and Mechanics, Graduate School of Engineering, 20 July 2012, KYOTO UNIVERSITY, Japan.

13. Kholmirzo KHOLOMURODOV, "Molecular Dynamics Simulations of Nano- and Biostructures", Scientific Seminar of Yasuoka Laboratory, Department of Mechanical Engineering, Faculty of Science and Technology, 24 July 2012, KEIO UNIVERSITY, Japan.


17. Roman Eremin, Kholmirzo Kholmurodov, Viktor Petrenko, Mikhail Avdeev, "Molecular dynamics simulations on pure cis- and trans-decalin solutions and their mixtures" XVI Conference of Young Scientists and Specialists (AYSS’12), 06 - 11 February, 2012, JINR, Dubna, Russia


**[Proceedings, etc.]**


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