Project Title:

Developments of computational tools to interpret low-resolution structural data

Name: ○Florence Tama, Osamu Miyashita

Laboratory at RIKEN: Computational Structural Biology Research Unit,
Computational Biophysics Research Team,
RIKEN Advanced Institute for Computational Science

1. Background and purpose of the project, relationship of the project with other projects

   Our research focuses on the development of computational tools to study biological systems, more specifically to help in the 3D structural determination of biological systems from various low-resolution experimental data (cryo-EM, XFEL) and to analyze their potential interactions with small molecules in order to design new drugs. Our target systems are large proteins and RNA molecular complexes and analyses of their structure and dynamics require large computational resources.

2. Specific usage status of the system and calculation method

   During FY2013, we have been developing algorithms to analyze XFEL data. After initial development of the tools on local workstations for smaller data set, we started to test large-scale calculations on RICC MPC from January. At RICC, we calculate similarities between a large number of imaging data using programs Xmipp and SPIDER with MPI.

3. Result

   The resulting data indicates that, while it is still preliminary, the similarity measurement programs can be used for XFEL data analysis. We will investigate the use of these programs further.

4. Conclusion

   We have been learning the computational environment at RICC, compiled programs, prepared some scripts for job submission and we have run some preliminary calculations.

5. Schedule and prospect for the future

   We would like to continue additional large-scale calculations on RICC. We will apply General Use category after we establish the tools and dataset for full calculations if the allocated CPU time is not sufficient.