Usage Report for Fiscal Year 2017

**Project Title:**

# High-precision trajectory calculation of cold ions

**Name:**
**Susumu Kuma, Sebastian Menk, and Shinji Okada**

**Laboratory at RIKEN:**
**Atomic, Molecular and Optical Physics Laboratory**

---

Investigation of molecular collisions and dynamics at low temperatures has been one of the important research areas in physics and chemistry. Recent experimental developments enable us to explore slow (long time-scale, extending to 1,000 sec) dynamics of molecular ions which is specific to such low energy processes.

Recently, we constructed a compact electrostatic ion storage ring named RICE (RIken Cryogenic Electrostatic ring). Low-energy collisions and reactions of cold molecular ions in the specific vibrational and rotational states prepared by the ring are our primary mission to be explored. Taking advantages that an electrostatic ring has no limitation of mass of stored ions, we expect that the excitation and de-excitation dynamics of large bio-molecular ions and cluster ions as well as energy-differential cross section of relevant collisions are revealed.

At the time of the application of this project, we aimed to numerically simulate molecular ion trajectories in the injection beam line to RICE using HOKUSAI. In particular, a quadrupole-type beam deflector, which bends ion beams from ion sources to RICE, required high-accuracy simulations of ion trajectories in the beam line. Because of the structural complexity of the quadrupole deflector, executions of charged-particle optics simulations were required using the supercomputing facility.

However, just after starting this project, we reconsidered the design of the beam line, and decided to construct a completely new cylindrical-type deflector. Due to its simple structure, we did not need to use HOKUSAI for charged particle optics simulations; instead, we successfully simulated the ion trajectories using a multi-CPU, server machine equipped in our laboratory. Experimental tests of this deflector will start within the FY.