# Development of reciprocal space mapping software for single crystal diffraction

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For crystal structure analysis including light weight atoms such as hydrogen and lithium and magnetic structure analysis for strong correlation system, neutron single crystal diffraction is very powerful tool. Generally, A two-dimensional area detector by X-ray and neutron diffraction has huge reciprocal space data, so that it is necessary efficient analysis method. In the past decade, we developed the program package "*Reciprocal Analyzer*", for a single crystal neutron diffractometer, using a curved two-dimensional position sensitive detector (C-2DPSD) installed at HANARO-ST3 and at T2-2 beam port in JRR-3M [1, 2]. This software was utilized by 32-bit OpenGL UI libraries "*GLUI*", and it realized cross-platform packages available used major operating systems. However, these user interfaces are old-fashion for present computers, so that it is essential to improve using recent libraries. Thus, we developed a new application based on three-dimensional reciprocal space mapping using latest C++17 languages, and it applied to TOF neutron data by neutron single crystal diffractometer "SENJU" installed at J-PARC/MLF shown in figure 1.

Moreover, we also developed UB matrix determination program based on probabilistic algorithm, which is bundled the reciprocal mapping software above mentioned. Some algebraic methods are well known as algorithms to calculate the UB matrix such as the two-reflection method and the vector minimum method. On the other hand, in many cases of samples brought to large neutron and Synchrotron experimental facilities, lattice parameters have already determined through preliminary experiments using laboratory X-ray equipment. Therefore, the determination of the UB matrix is often equivalent to the problem of finding the rotation matrix as U-matrix. Because the rotations in each axis are continuous variables and the number of combinations is proportional to the cube of the discrete rotations, the round robin algorithm is not a realistic solution. The Monte Carlo method is one of estimation methods for the global optimal solution by a probabilistic algorithm in a broad sense. In this study, we developed a UB matrix estimation program that newly introduced probabilistic algorithms such as (1) *Random Walk*, (2) *Simulated Annealing*, (3) *Generic Algorithm*, and (4) *Particle Swarm Optimization*, the properties and costs of each algorithm are discussed. In the presentation, we report the details of each algorithm and the comparison of the calculation results.

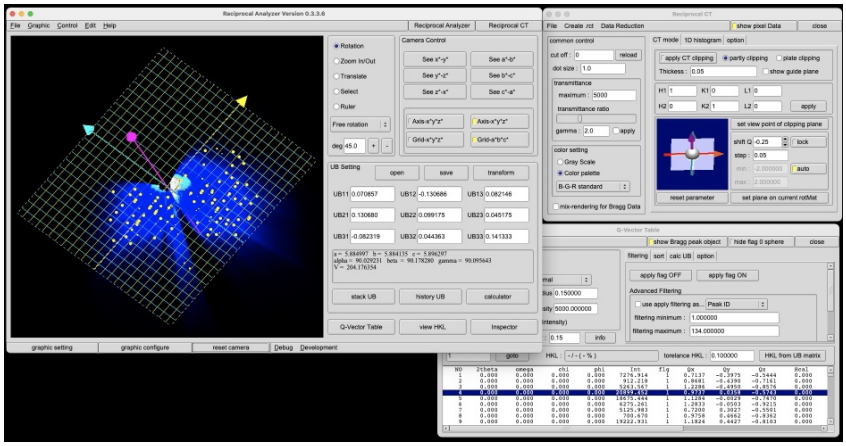

**Figure 1**. Reciprocal Space Mapping software "*Reciprocal Analyzer*".

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[2] Y. Noda, Y. Ishikawa, C-H. Lee, S. Kim, M. Moon (2011). *Acta Cryst.* ,**A67**, C652.

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