Neutron Macromolecular Crystallography at ESS

S. Aggarwal[1,3], J. Bergmann[1], A. Finke[2], D. Lundström[1], and E. Oksanen[1,3]

[1]Instruments Division, European Spallation Source ESS ERIC, P. O. Box 176, SE-221 00 Lund, Sweden

[2] European Spallation Source ERIC, Data Management and Software Centre, Asmussens Allé 305 DK-2800 Lyngby, Denmark

[3] Division of Computational Chemistry, Chemical Centre, Lund University, P.O. Box 124, S-22100 Lund, Sweden

The NMX Macromolecular Diffractometer at the European Spallation Source (ESS) is poised to benefit from the most powerful neutron source in the world. The ESS's long-pulse design is ideal for structural biology applications, including macromolecular crystallography. NMX, a time-of-flight (TOF) quasi-Laue diffractometer, is optimized for studying small samples and large unit cells, allowing precise location of hydrogen atoms critical to the function of biological macromolecules. It is projected that NMX at ESS could collect data from crystals as small as 200 µm within a few days, marking a significant improvement in both crystal size and data collection speed compared to current sources. The innovative robotic detector positioning system can accommodate large unit cells, resolving edges up to 300 Å, thereby expanding the range of biological molecules that can be studied using neutrons. This includes membrane proteins like proton pumps, positioning neutron crystallography to address a broader array of hydrogen-related questions in biomolecular science.

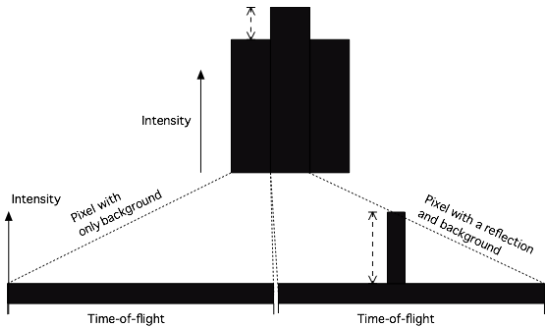


Figure 2: Spreading background over TOF

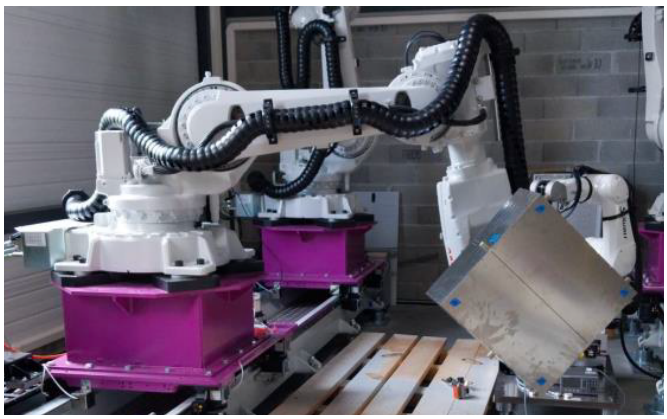


Figure 1: Detector positioning system for NMX