

NMX STAP Report (November 4, 2024)

The NMX STAP met on October 22-23, 2024, to receive updates on instrument construction and software development. Leighton Coates (Chair), Derek Logan, Kazuo Kurihara, John Helliwell, and Nobuo Niimura were present in person; Andreas Ostermann and Matthew Blakeley participated online.

The STAP was pleased to see that the incident neutron guide, choppers, and shutter on NMX have been installed and that progress is being made on the electrical installation within the instrument end station. However, the STAP feels that without significant effort to speed up the installation progress on NMX, its position within the tranche one instruments is unlikely to be realized. Also, the energization process at ESS is seen as a major risk across the LSS instrument suite, and NMX is no exception. Interaction with the Personal Protection Systems group was also seen as an issue that will affect NMX and several other instruments and will ultimately delay instruments being able to take first neutrons.

The STAP was impressed with the optimization work done on the GEM detector so far and highly supported testing of the detector at the DALI instrument beam of the ILL and especially its comparison with the neutron image plate type of detector installed there. This will provide valuable insights into the detector's performance using protein diffraction data, which is especially important as this detector has yet to be used on a neutron instrument anywhere in the world. Two essential requirements for the NMX detectors are positional resolution and detector efficiency. The low efficiency of the GEM detector (estimated at 10% and 30% respectively with unenriched and enriched Gd isotopes) continues to concern the STAP and will ultimately limit the scientific impact and productivity of the instrument. It will be essential to fully use existing resources and continue to improve the GEM NMX detector or to explore alternative existing detector technologies with significantly higher detector efficiencies and similar pixel sizes. It is perfectly acceptable for two different area detector technologies to be provided at NMX, ie the current one accommodating very large unit cells (up to 300Å), and another aiming at higher throughput for more medium range MX unit cells (up to say 150Å).

The STAP felt that ESS is wisely investing in optimizing the DIALS suite to process NMX data as an emerging standard software across the whole MX community. These efforts must likely continue for several years after the ESS beam on Target, as software testing with real data will only become available after NMX starts operations. DIALS has not been demonstrated to us to be able to reduce data from a neutron protein crystallography instrument, and we imagine that significant development will be required over the next few years.

The STAP felt that the support infrastructure to help users produce samples suitable for NMX is now in place and will allow new and existing neutron users to conduct experiments on NMX. This is currently a jewel in the crown of ESS activity we feel. Its role in developing new users will be vital though as the number of existing protein crystallography users within

the countries contributing to ESS is small although growing steadily. The STAP were pleased to see that the NMX team is being proactive in engaging with the protein crystallography community at an early stage such as the recent ECM Padova workshop that ESS organized, to start developing a broad user base for the NMX instrument.

Finally, the STAP feels ESS would greatly benefit from developing a resource-loaded schedule for instrument installation. Such a schedule would help define the number of key staff needed to realize the current schedule. Matching required to available resources will then help define an achievable schedule for completing NMX instrument installation.