

## MX PReSTO 2019

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In 2013, Protein Science Facility (PSF) from Karolinska Institutet in Stockholm and National Supercomputer Centre (NSC) in Linköping, started a pilot project to evaluate performance of Macromolecular X-ray crystallography (MX) applications running in an HPC environment. In 2015, the Swedish light source MAX IV decided to fund a pilot extension called PReSTO (<https://www.nsc.liu.se/support/presto/>), that aim to support integrated structural biology calculations including MX, Nuclear Magnetic Resonance (NMR) and cryo-electron microscopy (cryo-EM). During 2017-2018 the MX-PReSTO installation was made using easybuild with several advantages to a standard HPC installation such as

- A) software environments can be send to compute nodes
- B) software dependencies are visible in easyconfigs.

In 2018, the Swedish Research Council granted funds (dnr. 2018-06479) to a collaborative extension of MX-PReSTO towards Cryo-EM/SciLifeLab and NMR/Swedish NMR Centre. Now in 2019, the MX-PReSTO installation will be placed under version control and in September 2019, we want to share easy-build daily maintenance and operations with local HPC administrators at the MAX IV site. Swedish researchers visiting BioMAX receive some MX-HPC training during beamtime. Regular after beamtime training sessions with users own data/questions will be available at weekly drop-in sessions at protein science facility, Karolinska Institutet. Startup PReSTO seminar or workshop can also be requested by all Swedish Universities by contacting Martin Moche as done by UU in 2015 and SLU in 2018.

Access to the PReSTO installation is via Swedish National Infrastructure of Computing (SNIC) funded by the Swedish Research Council. Thinlinc is a remote desktop server from Cendio that supports the integrated structural biology workflow by enabling graphic applications i.e. coot/chimera/ccp4mg/pymol to run smoothly from a remote computer. The homepage (<https://www.nsc.liu.se/support/presto/>) is written for HPC-MX newcomers showing how to interact with the HPC setup by loading modules, request compute time, core and nodes, writing sbatch scripts, schedule and monitor jobs, describe how to use PHE-NIX with slurm scheduling, and pointing towards many MX software developer manuals. To adapt new users to the MX-HPC workflow we also developed a helpful PReSTO menu that

- A) launch MX software at login or compute node with graphics support
- B) enable user to select number of cores and runtime at compute nodes
- C) enable user to select output directory for software such as hkl2map.

PReSTO for MX is now available at NSC Tetralith, LUNARC Aurora and the MAX IV cluster. Please acknowledge SNIC (<https://www.snic.se/allocations/apply4access/>) when using its resources.