

PReSTO: Structural Biology Software in a High Performance Compute Environment

PReSTO is a software stack for integrated structural biology adapted to high performance computing resources at the Swedish National Infrastructure for Computing (SNIC) and the local MAX IV compute cluster. Our aim is to support integrative structural biologists evaluate their data from macromolecular X-ray crystallography (MX), X-ray free electron lasers (XFEL), nuclear magnetic resonance spectroscopy (NMR), cryo-electron microscopy (cryo-EM), neutron scattering (NMX), and small-angle X-ray scattering (SAXS). The purpose of PReSTO is to provide users with convenient access to useful software already set up and optimized for powerful supercomputing platforms. The PReSTO team supports software updates and bugs and assists users by facilitating access to the various platforms we support.

Primary authors: ACEBES, Marcos (Lund University); AHLNER, Alexandra (Linköping University); AURELIUS, Oskar (MX); FINKE, Aaron; GONZALEZ, Ana (MAX IV); HÖRNELL, Karl (National Supercomputing Centre); LUCKEY, Christian (National Supercomputing Centre); MATEJ, Zdenek; MOCHE, Martin (Karolinska Institutet); NAN, Jie (MX-group); RASMUSSEN, Torben (National Supercomputer Centre); SJÖSTRÖM, Anders (Lund University); SUNNERHAGEN, Maria; THORARENSEN, Sebastian (National Supercomputing Centre)

Presenter: FINKE, Aaron