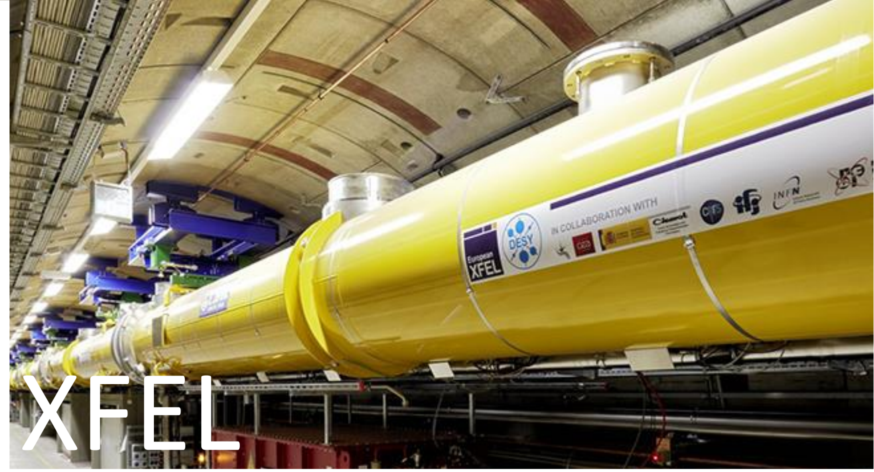
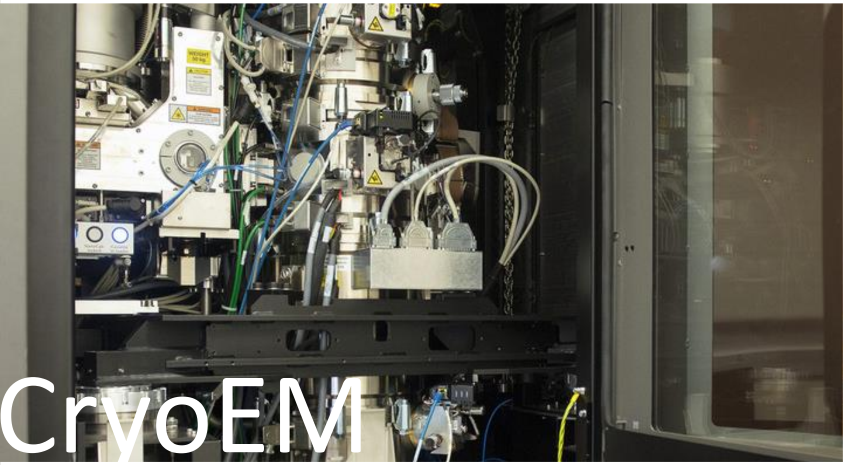
NMR

NMX



XFEL



CryoEM

MX

PReSTO – structural biology software in HPC environment

Status report June 2021

PReSTO history

2013

National Supercomputer Centre (NSC) visits Tällberg

2015

PReSTO gets MAX IV satellite status

2016

Software deployment tool Easybuild introduced

- Version control/testing, explicit dependencies, hardware transfer simplified

2018

Funding from Swedish Research Council (ends 2022)

- Involve Cryo-EM, NMR and XFEL (serial crystallography)

2020

SNIC storage project

Software in PReSTO – June 2021

MX (XDS, CCP4, PHENIX, GlobalPhasing, PyMOL, ChimeraX, USF)	tbd: Python2->Python3 transfer, DIALS3, CCP4 v.7.1, CSD, automated testing
XFEL (CrystFEL, Cheetah, nXDS)	tbd: cctbx-xfel, DatView
Cryo-EM (Scipion, Relion, CisTEM, EMAN2, Gctf, Gautomatch, Motion2Cor, CTFFIND)	tbd: CryoSPARC, CryoDRG, eTomo, Dynamo, EMClarity, PEET,..
NMR (NMRPipe, MddNMR)	tbd: CS_Rosetta, Catia, PINT, CYANA, FLYA, ARIA,..

PReSTO usage June 2021

	MX	XFEL	CryoEM	NMR
infrastructure	**MAX IV**	**MAX IV**	**SciLifeLab**	**SNC**
community	**YES**	**YES**	**NO**	**NO**
reason	**available**	**available**	**data transfer**	**too few sw**


MAX IV


LUNARC


NSC Berzelius


NSC Tetralith

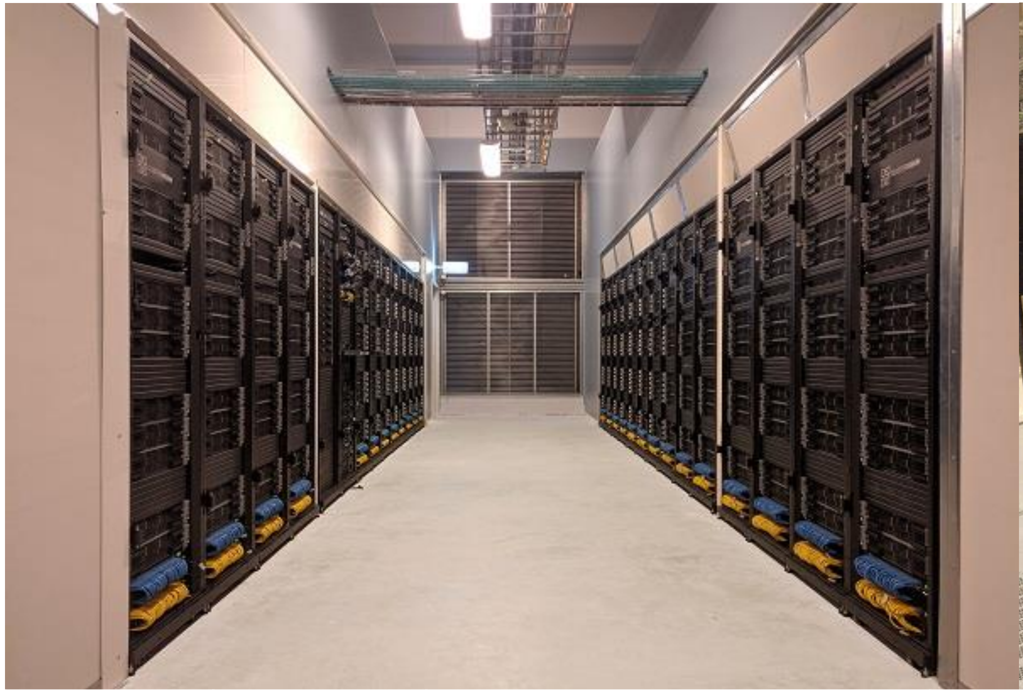
Hardware with PReSTO today and tomorrow

PReSTO at MAX IV

MAX IV cluster divided into → online@beamtime
→ offline@home

- online/offline clusters share PReSTO installation
- offline cluster PReSTO use without data transfer
- online data processing (NO PReSTO)
- build FragMAXapp on top of PReSTO

NSC Tetralith (2018) vs Berzelius (2021) GPU nodes



NSC	Nodes	CPU type	CPUs	RAM	GPU	/scratch/local
Tetralith	170	2x Intel Xeon Gold 6130	32	96 GiB	1 NVIDIA® T4	2 TB NVMe SSD
Berzelius	60	2 AMD Epyc™ 7742	128	1 TB	8 NVIDIA® A100 Tensor Core	15 TB NVMe SSD

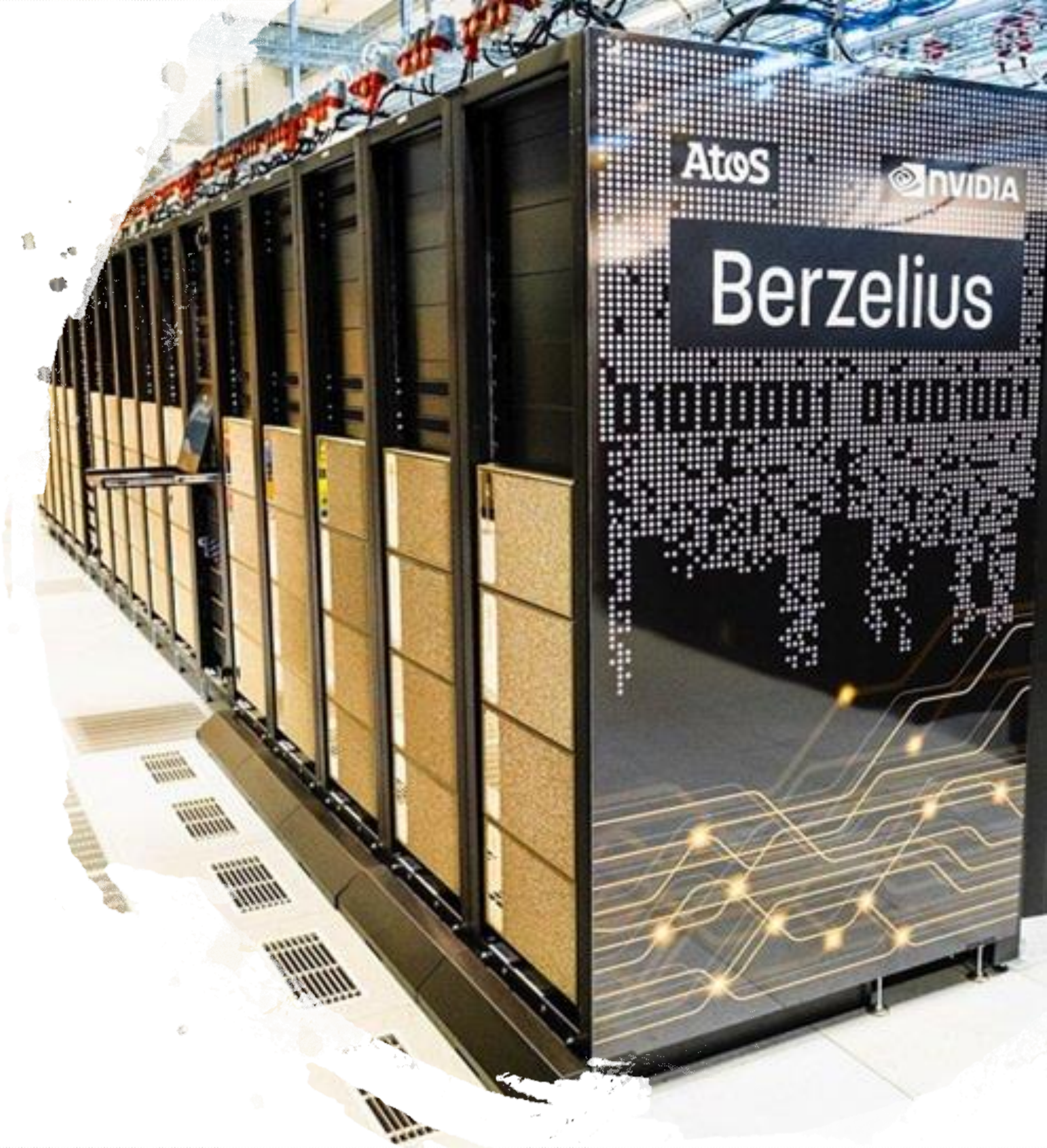
Gitlab and easybuild simplifies moving PReSTO to new hardware

Cryo-EM PReSTO at Berzelius

Researchers not using AI/ML methods may apply provided

- ✓ Their project show efficient NVIDIA GPU use by their software
- ✓ NSC support for non-AI/ML workflows will only be provided if time allows
- ✓ Outside of the focus area of Berzelius, no special compute environment or software are supported by NSC
- ✓ The researcher must be able to manage their own software stack

https://www.nsc.liu.se/support/systems/resource-allocations-on-berzelius/



PReSTO support and training…

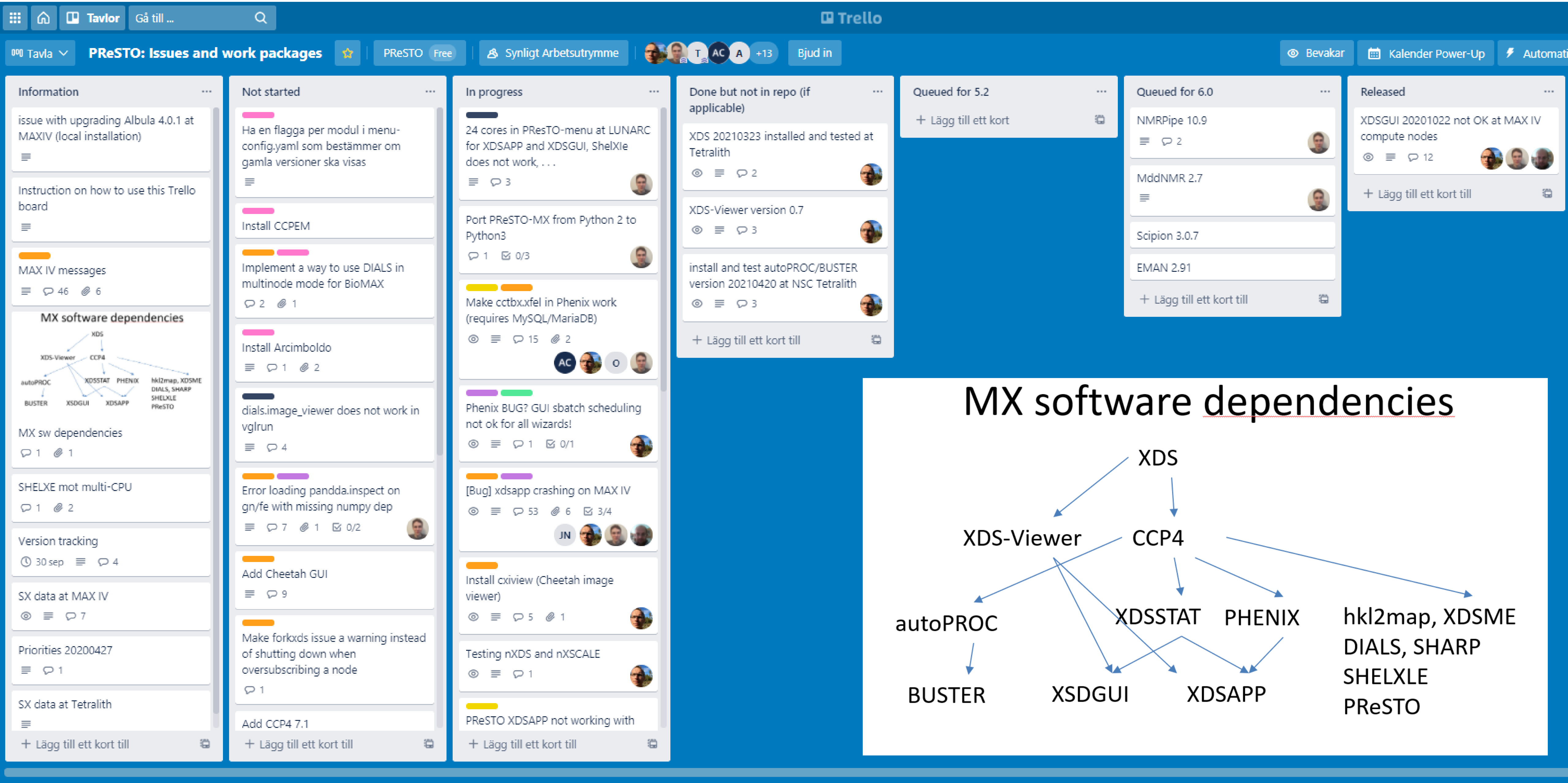
PReSTO homepage(MX only)

- https://www.nsc.liu.se/support/presto/
- MX software and CrystFEL startup scripts
- Phenix GUI slurm configuration
- Login vs compute nodes

MX trainee requires

- Own data to analyze
- User account on SNIC/MAX IV cluster with PReSTO
- Multiple 2-hour zoom sessions until saturation/satisfaction
- https://www.nsc.liu.se/support/presto/MX-PReSTO%20training/

Trello for project management



Information

- issue with upgrading Albula 4.0.1 at MAXIV (local installation)
- Instruction on how to use this Trello board
- MAX IV messages — 46, 6
- MX sw dependencies — 1, 1
- SHELXE mot multi-CPU — 1, 2
- Version tracking — 30 sep, 4
- SX data at MAX IV — 7
- Priorities 20200427 — 1
- SX data at Tetralith
- + Lägg till ett kort till

Not started

- Ha en flagga per modul i menu-config.yaml som bestämmer om gamla versioner ska visas
- Install CCPEM
- Implement a way to use DIALS in multinode mode for BioMAX — 2, 1
- Install Arcimboldo — 1, 2
- dials.image_viewer does not work in vglrun — 4
- Error loading pandda.inspect on gn/fe with missing numpy dep — 7, 1, 0/2
- Add Cheetah GUI — 9
- Make forkxds issue a warning instead of shutting down when oversubscribing a node — 1
- Add CCP4 7.1
- + Lägg till ett kort till

In progress

- 24 cores in PResTO-menu at LUNARC for XDSAPP and XDSGUI, ShelXle does not work, . . . — 3
- Port PReSTO-MX from Python 2 to Python3 — 1, 0/3
- Make cctbx.xfel in Phenix work (requires MySQL/MariaDB) — 15, 2 — AC, O
- Phenix BUG? GUI sbatch scheduling not ok for all wizards! — 1, 0/1
- [Bug] xdsapp crashing on MAX IV — 53, 6, 3/4 — JN
- Install cxiview (Cheetah image viewer) — 5, 1
- Testing nXDS and nXSCALE — 1
- PReSTO XDSAPP not working with
- + Lägg till ett kort till

Done but not in repo (if applicable)

- XDS 20210323 installed and tested at Tetralith — 2
- XDS-Viewer version 0.7 — 3
- install and test autoPROC/BUSTER version 20210420 at NSC Tetralith — 3
- + Lägg till ett kort till

Queued for 5.2

- + Lägg till ett kort

Queued for 6.0

- NMRPipe 10.9 — 2
- MddNMR 2.7
- Scipion 3.0.7
- EMAN 2.91
- + Lägg till ett kort till

Released

- XDSGUI 20201022 not OK at MAX IV compute nodes — 12
- + Lägg till ett kort till

MX software dependencies

How can you support PReSTO?

1. Use PReSTO!
   report BUGs to SNIC support (or PReSTO team members)
2. Suggest software to be added into PReSTO
   What is most important NMR/Cryo-EM/XFEL package to add?

3. Perform software updates (require PReSTO admin rights)
   Free up time for PReSTO staff to deal with new installs and issues
4. Add new software to PReSTO (require PReSTO admin rights)
   PReSTO to educate interested community representatives

PReSTO acknowledgements

Lima, G.M.A. et al. FragMAXapp: crystallographic fragment-screening data-analysis and project-management system. *Acta Crystallogr D Struct Biol* **77**, 799-808 (2021).

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Brock, J.S. et al. A dynamic Asp-Arg interaction is essential for catalysis in microsomal prostaglandin E2 synthase. *Proc Natl Acad Sci U S A* **113**, 972-7 (2016).

Janfalk Carlsson, A. et al. Laboratory-Evolved Enzymes Provide Snapshots of the Development of Enantioconvergence in Enzyme-Catalyzed Epoxide Hydrolysis. *Chembiochem* (2016).

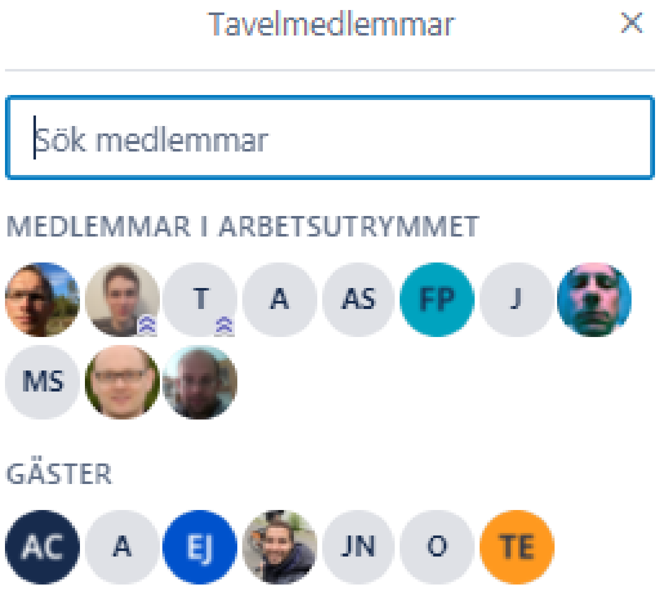
PReSTO team acknowledgement

Sebastian Thorarensen
Torbjörn Lönnemark
Filip Polbratt
Karl Hörnell
Anton Haglund
Torben Rasmussen
Johan Raber

NSC

Anders Sjöström

LUNARC



Tavelmedlemmar

Sök medlemmar

MEDLEMMAR I ARBETSUTRYMMET

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MAX IV