

ROCK-IT

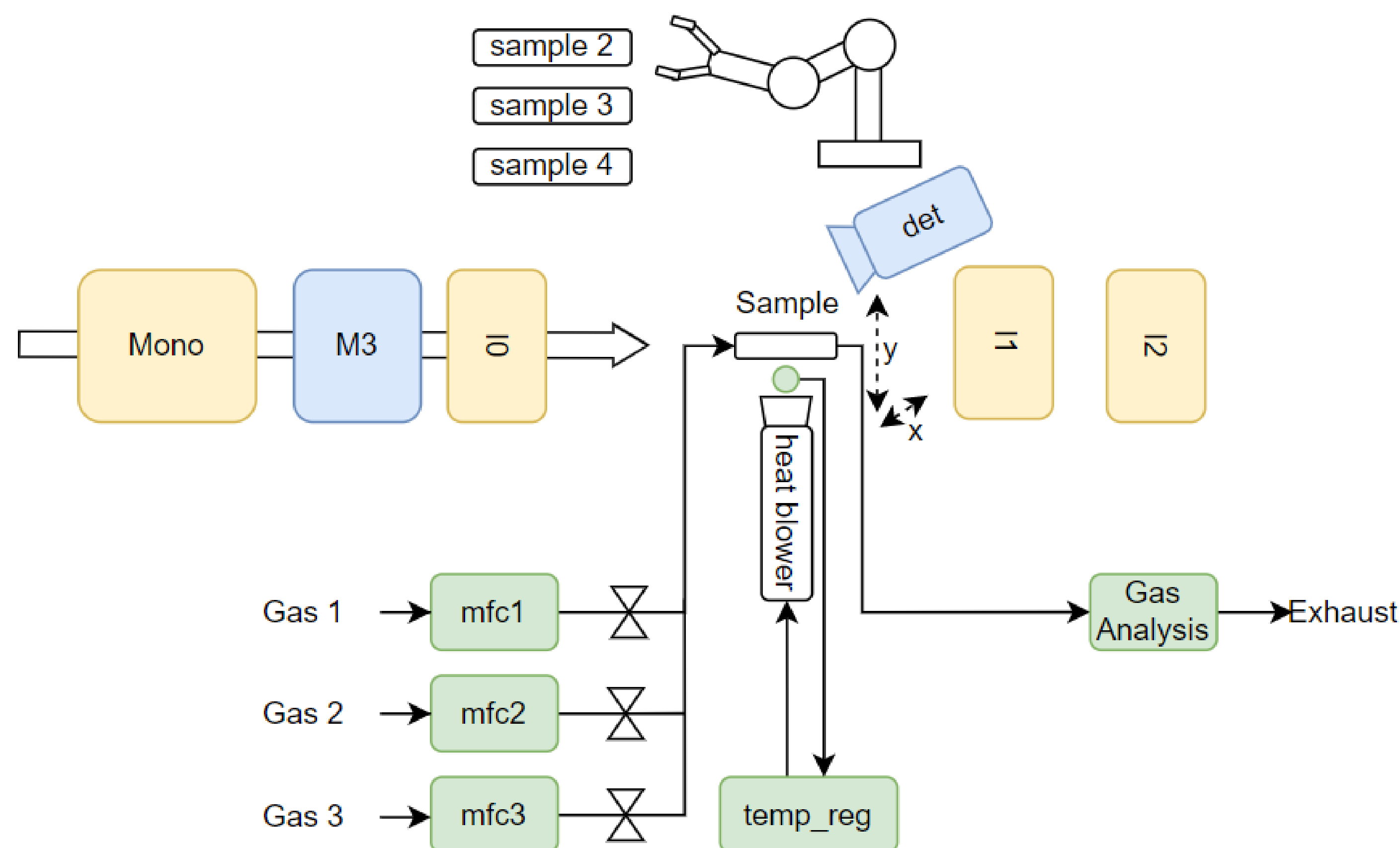
Beamline and Experiment Control

Will Smith Helmholtz-Zentrum Berlin GmbH on behalf of the other members of ROCK-IT WP2 from HZB, HZDR, KIT and DESY

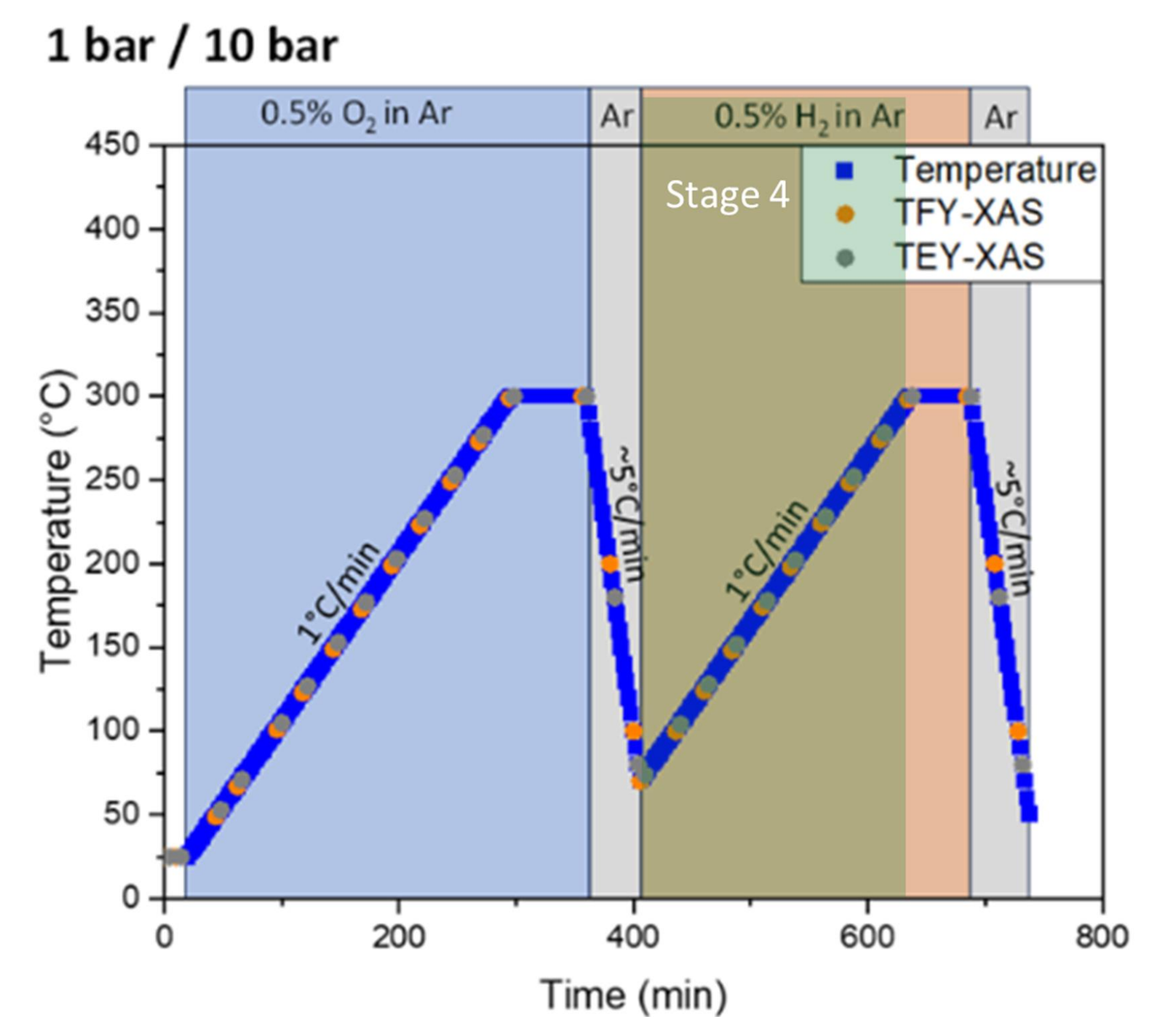


CONTROLLING OPERANDO EXPERIMENTS

Operando catalysis experiments involve many different devices. The sample environment changes over the course of hours while measurements are taken repeatedly with the X-Ray beamline to study the material. All of the data needs to be correlated together at the end. This presents a major challenge from a control, user interface and data management perspective. ROCK-IT aims to tackle this problem. Spanning 4 facilities with slightly different use cases and different field layers (Tango, EPICS, SECoP), Ophyd is used as a common interface layer allowing for cross facility solutions to be developed on top.



Experiment Split into Stages



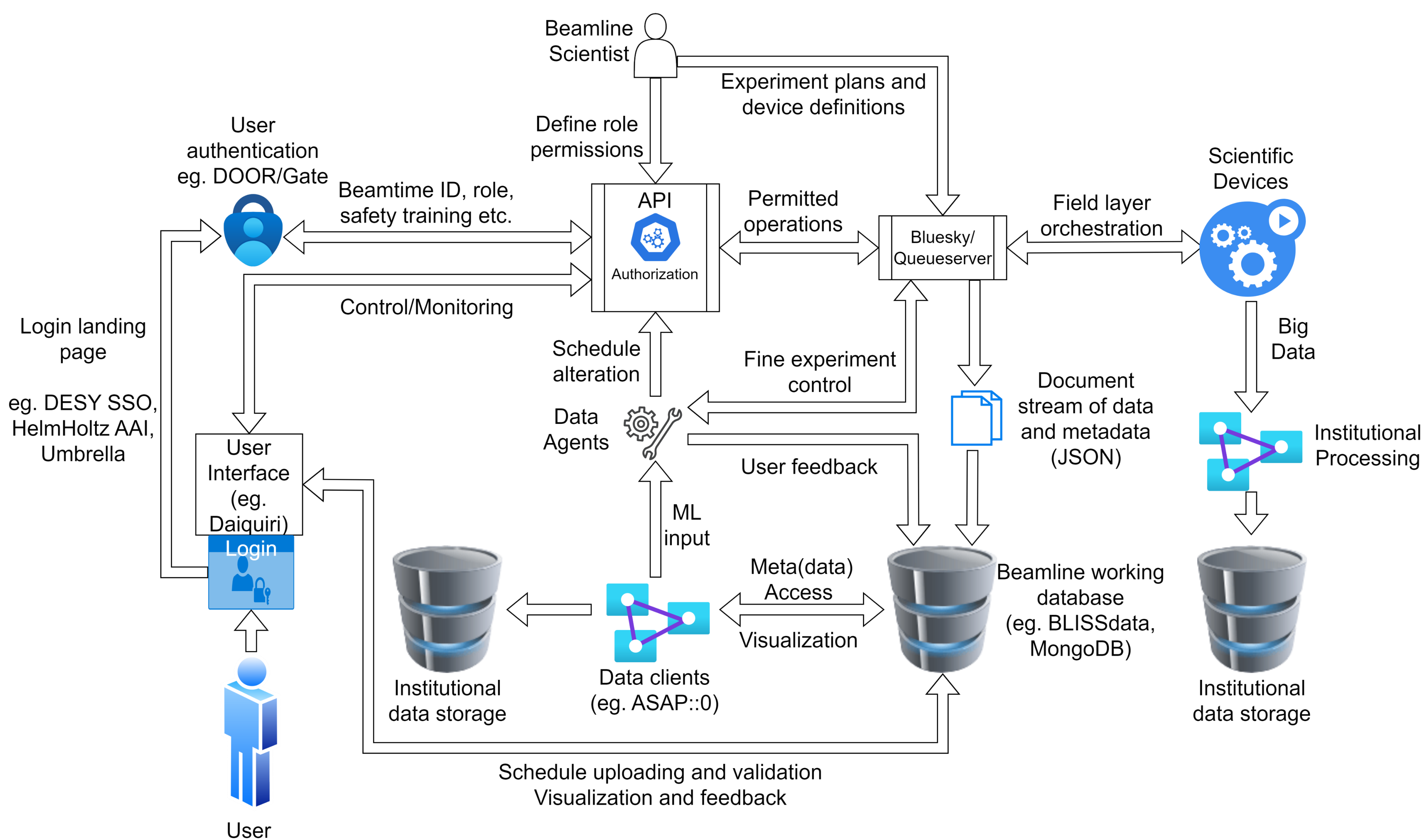
Each stage defines a specific gas mixture and temperature ramp or dwell as well as the requested photon measurements to be performed during that stage. For example EXAFS or XRD which should be run in a loop with some delay.

ALLOWING FOR EXPERIMENT MODIFICATION ON THE FLY

In the ideal case the user defines the experiment that should be performed on each sample and then leaves it to run unattended. In practice things go wrong or assumptions change and the experiment needs to be changed. The Bluesky Queueserver allow for these changes to be made by either human or AI agent while the experiment is still running. This makes fully autonomous operando catalysis experiments possible.

Stages Represented as Bluesky Plans

Each stage is represented as a Bluesky plan. These plans are executed sequentially by the Bluesky Queueserver. Participating institutes in ROCK-IT are attempting to share well tested plans between them.



Automated Export to NeXus App Def.

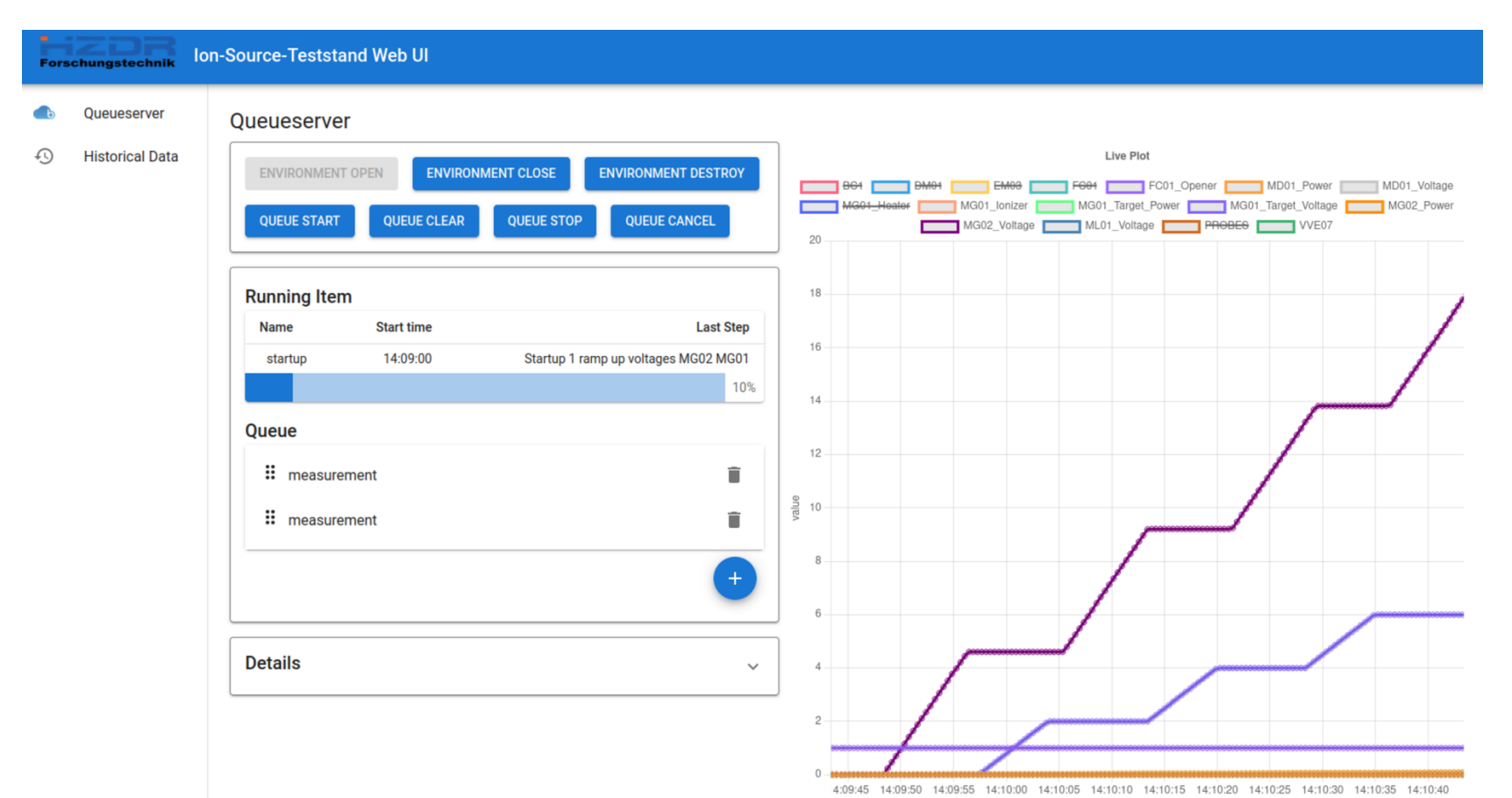
By collecting metadata about devices using Ophyd and Bluesky including their NeXus class it is possible to automatically export a NeXus file containing a populated NXinstrument entry.

By collecting additional metadata about the technique(s) and user it becomes possible to export NeXus application definition files.

ROCK-IT aims to address this problem consistently at each participating institute. See the poster of Sonal Patel at Poster #62.

This infrastructure interacting with EPICS, Tango or SECoP devices through Ophyd and running plans with a Bluesky Queueserver is common among all four of the participating institutes. Regular meetings and a common set of tools has helped to foster extensive collaboration.

User Interface



All participating institutes are using web based UI using REACT to control their Bluesky Queueserver and experiment with the aim of facilitating platform independent remote access. Here is a REACT based UI from HZDR.

ACKNOWLEDGEMENTS

We gratefully acknowledge funding from the Helmholtz Association HGF for the ROCK-IT project.