A shared vision for macromolecular crystallography over the next five years

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Macromolecular crystallography at synchrotron sources has reached a critical juncture. New diffraction-limited storage rings and upgrades to existing sources will provide beamlines with higher flux and brilliance, even the largest detectors can now collect at rates of above 100 Hz, and electron cryo-microscopy is successfully competing for structural biologists' most exciting projects. As a result, formerly scarce beam time is becoming increasingly abundant, and beamlines must reinvent themselves to attract users and ensure continued funding. Together with the audience, we want to explore what macromolecular crystallography at synchrotrons might look like in three to five years.

We will show how data collection has changed over the last decade and how improved algorithms have made it possible to collect significantly more pixels per unit time without adding to the compressed data rate. We will present current best practices for collecting, processing and archiving diffraction data and show how they will evolve with the latest generation of X-ray detectors. An important question for synchrotron beamlines is what metadata we need to ensure long-term archivability of diffraction data? During the last five years, an image-centric view of data collection has been replaced by a dataset-centered view. Instead of one CBF file per image, a few HDF5 files per dataset are now saved and processed. How will the community handle the switch to HDF5 1.10, which is not fully compatible with the earlier version used by EIGER detectors?

In the future, serial crystallography will further rise in prominence. Not only does it yield structural information from small and weakly diffracting crystals but it also supports the study of structural polymorphs and dynamics. What changes are required in hardware and software to support this development?