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Real-time data processing for serial X-ray crystallography at PETRA III

We have implemented a system for fully real-time data processing during a serial X-ray diffraction experiment, with (in principle) no need to store image data on disk. Using the CrystFEL software in combination with the ASAP::O data framework, frames from a 16 megapixel Dectris EIGER2 X detector were searched for peaks, indexed and integrated at the maximum full-frame readout speed of 133 frames per second. The pipeline produced un-merged Bragg reflection intensity measurements which could be directly scaled and merged in order to solve the structure.

By carefully optimizing the analysis software and processing parameters, we have been able to reduce the amount of CPU power needed to keep up with the data flow. Whereas around 1,800 cores were needed on our first attempt, now only around 24 are required. This contribution will discuss what we learnt from this process, and touch on the possible implications for experimental design.

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