# Serial crystallography

Real-time data processing for serial crystallography at P11

Thomas White and Tim Schoof DESY Photon Science Computing Workshop 10 Nov 2023

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES











# Serial crystallography experiment setup



 $\rightarrow$  One exposure per crystal

- → Steady stream of crystals
- $\rightarrow$  Each image processed independently
- $\rightarrow$  A lot of images (millions) (5 GB / sec, 100 TB per expt)
- $\rightarrow$  Data processing after experiment (months, even years!)

# **Processing pipeline**





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### **Processing pipeline**



### **Benefits of real-time data processing**

- $\rightarrow$  Faster results and publication
- → No need to store raw data (BIG cost reduction)
- $\rightarrow$  Better situational awareness during experiment
- $\rightarrow$  Faster diagnosis of experiment problems
- $\rightarrow$  Less scope for self-delusion

### Profiling graph



Frame number

malloc-copy asapo-fetch seedee-panel flag-values pf8-mask pf8-rstats pf8-search peak-search asdf-triplets asdf-findcell asdf-search integration other zero-mask process-image root

- asapo-get-next seedee-deserialize load-image-data prerefine-cell-check