

PAUL SCHERRER INSTITUT



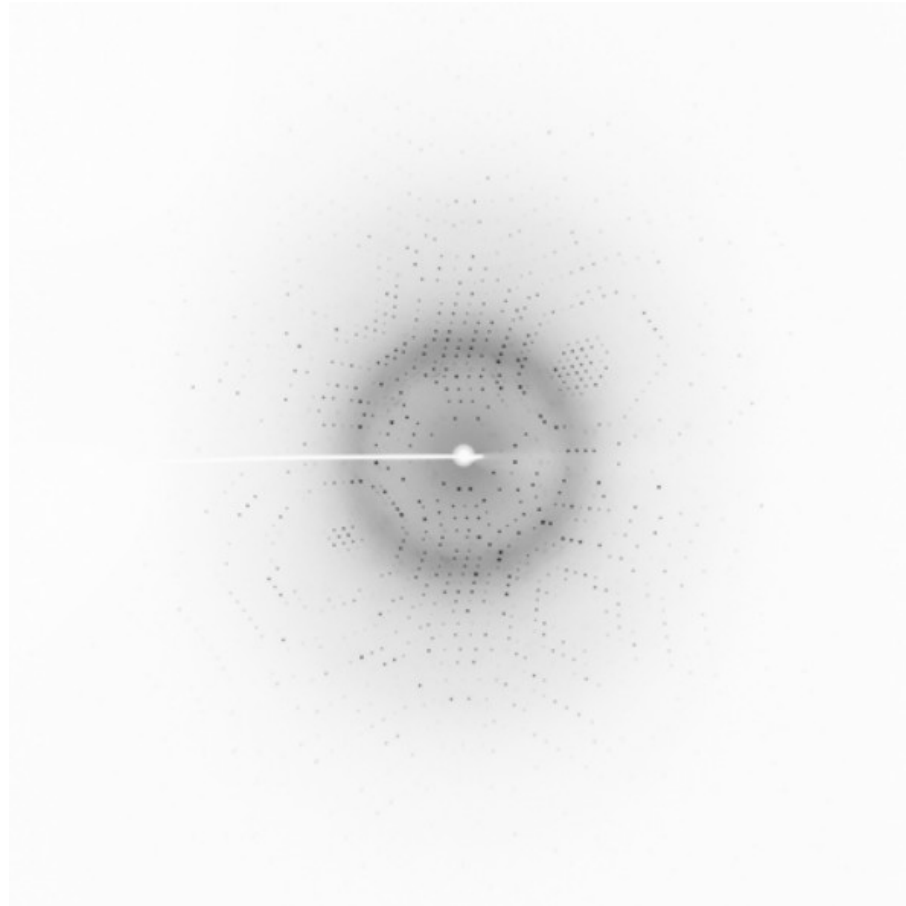
HC Stadler :: HPC Developer :: Paul Scherrer Institute

Proteine Crystallography – Spot Finding and Indexing for fast Experiment Feedback

JungfrauMX Project for SLS 2.0 lead by Filip Leonarski

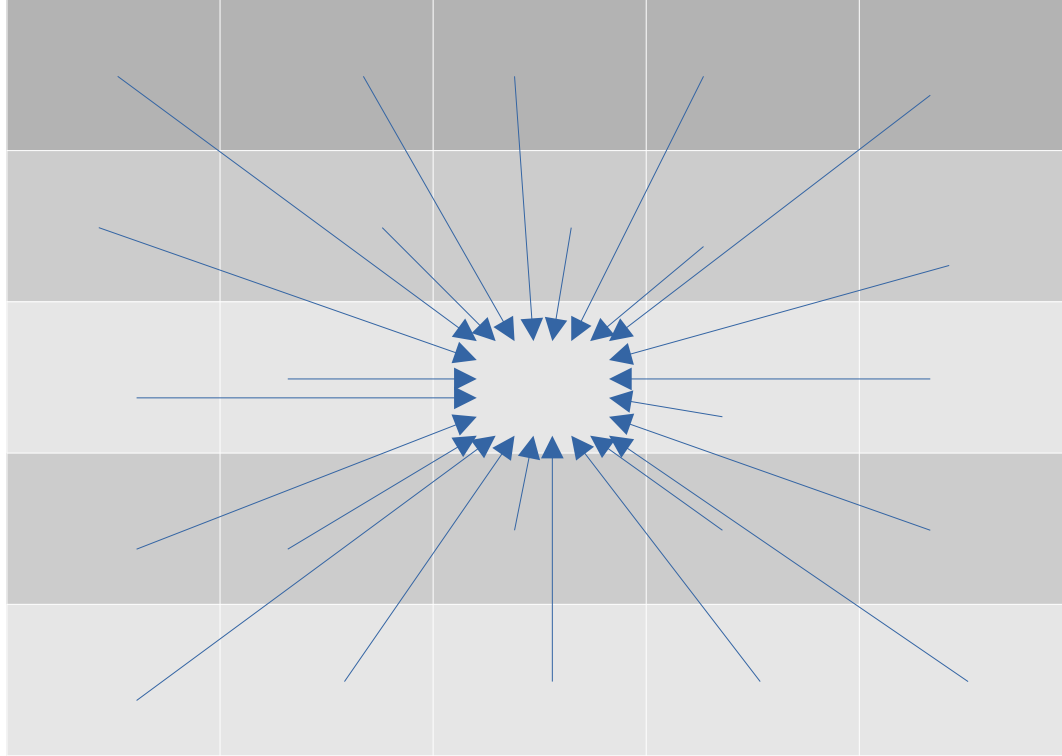


Raw Data

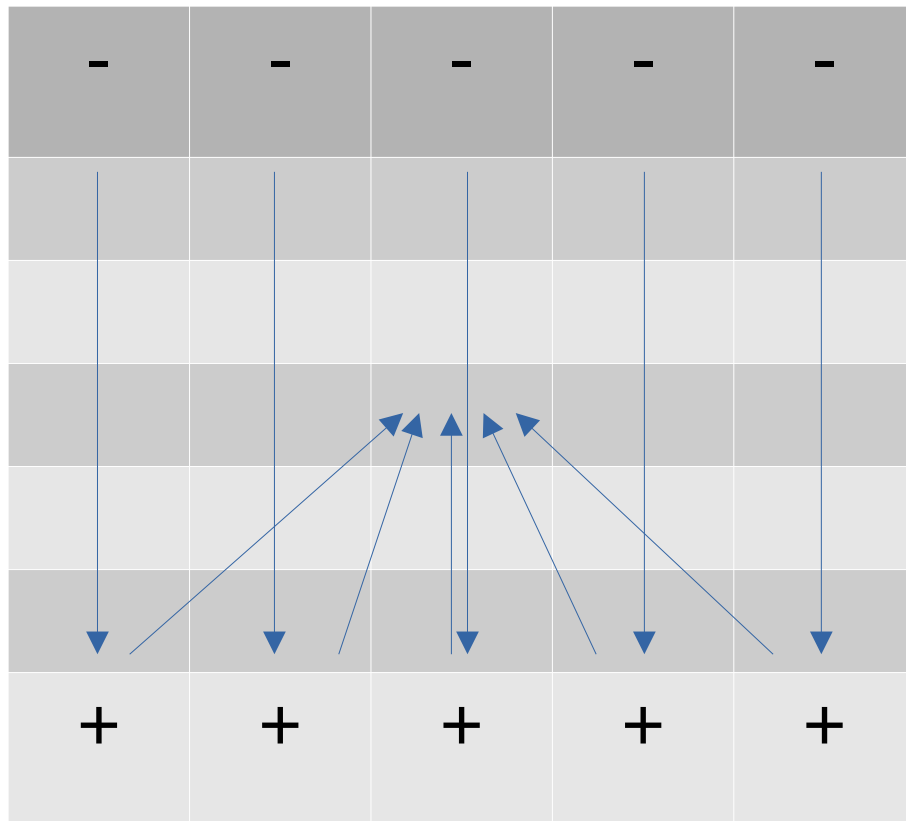


- Find spots in the detector signal
 - Detector pixel values significantly different than the surrounding values are candidates
 - Colspot algorithm: find candidates using mean and variance of a sliding window
 - Fast feedback means compute time less than 1ms
- Filip Leonarski implemented a GPU version of colspot – too slow
- Algorithmic improvements leading to lower GPU memory bandwidth consumption
 - 4x speedup – fast enough

Original Colspot Kernel

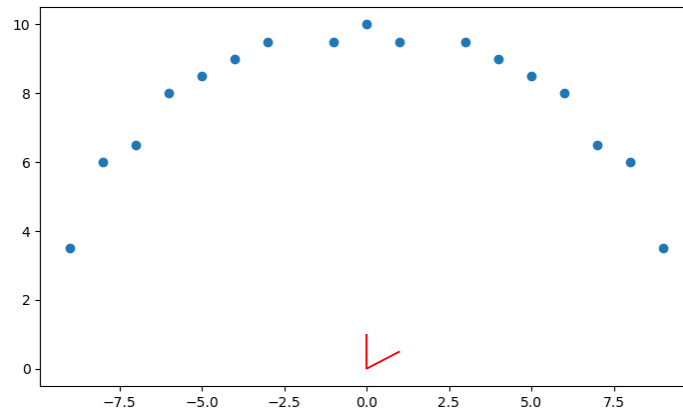
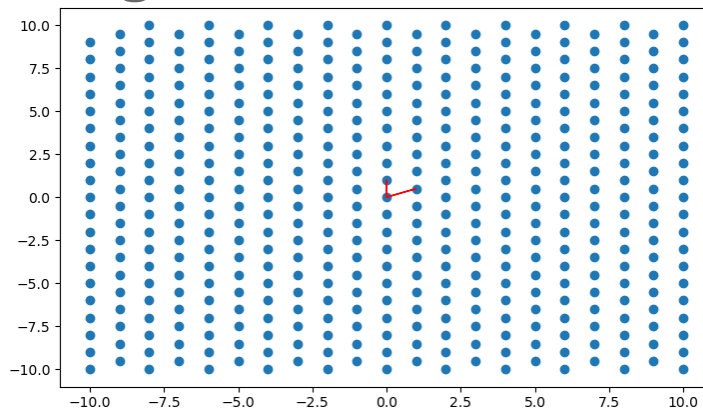


Faster Colspot Kernel – Wave Top to Bottom



- Find generating vectors of a grid
 - Fast feedback means compute time as close to 1 ms as possible
- Existing Xgandalf algorithm: single core code – too slow
- Attempting to implement existing dials indexer on GPU
 - Collaborate with Graeme Winter + Co

Indexing Problem in 2D (3D in reality)



Summary:

Make fast feedback for spot finding and indexing possible in the context of the new Jungfrau detector.

