

PSI Center for Scientific Computing,
Theory and Data

AWI Department Update

Overview of Group 7902

Markus Janousch for 7902
PSI, 27 May 2024

DataProcessing and Development Group (7902)



We work hand in glove with scientist and user communities to develop and support data reduction and processing software tools on the most appropriate platforms to meet their experiment and data analysis needs.

We offer domain expertise bridging both scientific disciplines and cutting-edge technologies to open new opportunities and horizons. We bring skills, expertise and knowledge to allow research scientist to focus on the scientific challenge.



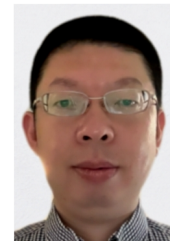
**Alain
Studer**



**Hans-
Christian
Stadler
Kleeb**



Ivan Usov

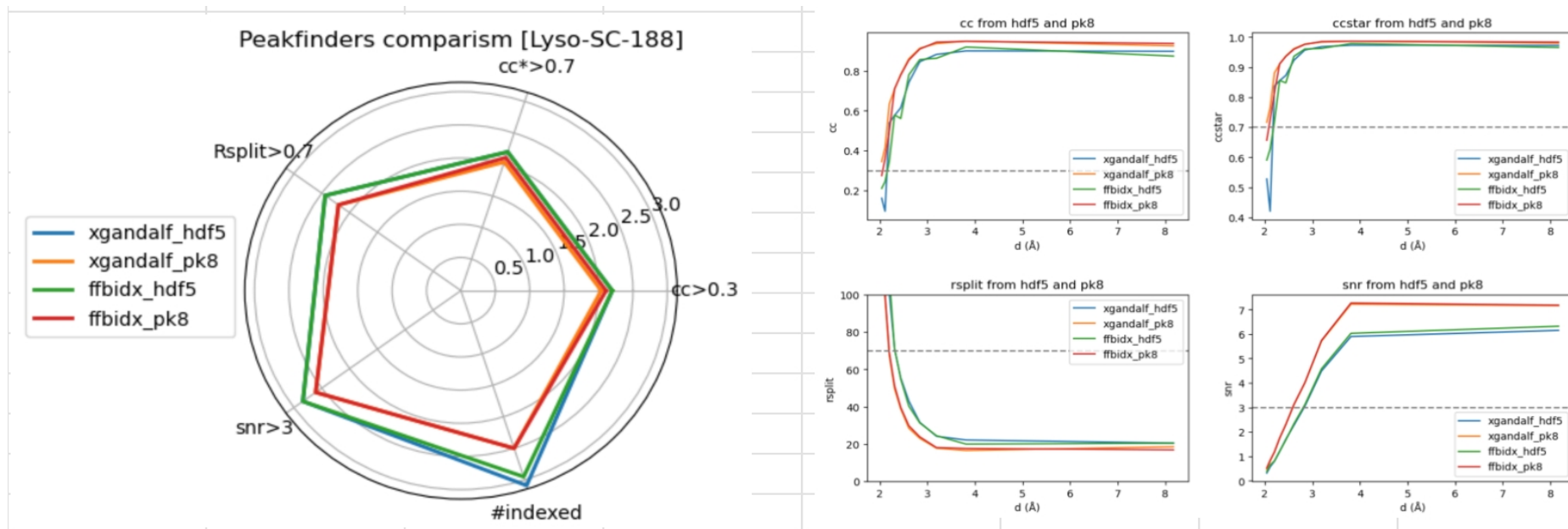


Jun Zhu



**Markus
Janousch**

JungfrauMX (HC)



First quality results for CUDA implementation of the new indexer look good (Jiaxin Duan)

RED-ML published (<https://doi.org/10.1107/S1600576724003182>)

TimePix 3 Detector (HC)

Initial implementation too slow (factor 20)

Bottleneck (lock protecting a histogram) identified and replaced by thread local histogramming with less frequent aggregation into final histogram

Probably a few more optimization rounds required

TOMCAT Reconstruction Pipeline: Scalability Test (Alain)

Motivation: New Detector of size 4k x 4k pixels

Using techniques such as stitching, stacking or zero-padding, virtual detector size up to 8k x 8k standard detector size is 2k x 2k

Scaling Characteristics and Design Goal

Raw data size increases by factor ~ 10 if number of pixels is doubled (in one dimension)

Detector dimension: $2k \rightarrow 4k \rightarrow 8k$

Increase in input size: $1 \rightarrow 10 \rightarrow 100$

Goal: Runtime should remain approximately constant if resources are scaled accordingly

TOMCAT Reconstruction Pipeline: Scalability Test (contd)

2k: Input size 16 GB, reconstruction time 100s on 1 node, ~20 cores @Ra

4k: Input size 160 GB, reconstruction time 100s on 2 nodes, ~200 cores
@Eiger

8k: Input size 1.6 TB, reconstruction time 200s on 20 nodes, ~800 cores
@Eiger

BEC Deployment (Ivan)

Work together with Boris, Ivano, and Leo

Automatic deployment of standard BEC components through Ansible.
Tests at three different beamlines (microXAS, PX, and Debye) so far.

Pyzebra (Ivan)

Migration from RH 7 to RH 8. Some refinement of the code base.

Deployment is now fully automatized.

Training

Basic Python training now available at PSI. One course from MIT course (free) and one paid (still needs set-up).

Work on a knowledge base started.