FS computing 2023

Report of Contributions

https://indico.desy.de/e/42131

Contribution ID: **2** Type: **Short talk**

Data reduction activities in FS-DS (photon science detector systems)

Friday 10 November 2023 11:45 (15 minutes)

New detectors produce increasing volumes of data, and so performing data reduction close to the detector (e.g. on detector-specific data acquisition PCs) can potentially reduce the workload on later infrastructure. I will present on current work on this in FS-DS. Also, for historical reasons, FS-DS are responsible for the DESY part of a few collaboration projects on data reduction: Data-X, HIR3X workpackage 2, and LEAPS-INNOV workpackage 7. I will present these projects, and we can discuss how to proceed with them in future.

Primary author: PENNICARD, David (FS-DS (Detektorsysteme))

Presenter: PENNICARD, David (FS-DS (Detektorsysteme))

Contribution ID: **3** Type: **Poster**

Real-time data processing for serial crystallography at P11

Friday 10 November 2023 12:30 (5 minutes)

We have been using ASAP::O to process data in real time from an Eiger 16M detector, in serial crystallography experiments at P11. The system performs a peak search before indexing and integrating each diffraction pattern, producing Bragg reflection intensity measurements without any need (in principle) to store image data.

Through rounds of performance profiling, we reduced the time taken to process one pattern (in one thread) to only 455 ms, meaning that the dedicated P11 computing resources are sufficient to keep up with the 133 frames per second speed of the Eiger detector, despite the very large number of pixels (16M).

The pipeline is available for user experiments at P11 (and other beamlines).

Primary author: Dr WHITE, Thomas (FS-SC)

Co-authors: TOLSTIKOVA, Aleksandra (FS-SC Photon Science Scientific Computing); HENKEL, Alessandra (FS-CFEL-1 (Forschung mit Photonen Experimente 1)); Dr GRUZINOV, Andrey (DESY); Mr KLOPPROGGE, Bjarne (FS-PS (Photon Science)); OBERTHUER, Dominik (FS-CFEL-1 (Forschung mit Photonen Experimente 1)); POMPIDOR, Guillaume (DESY); TABERMAN, Helena (FS-PETRA-D (FS-PET-D Fachgruppe P11)); MEYER, Jan (FS-CFEL-1-BMX (FS-CFEL-1 Fachgruppe BMX)); HAKANPAEAE, Johanna (FS-PETRA-D (FS-PET-D Fachgruppe P11)); HANNAPPEL, Juergen (IT (IT Scientific Computing)); GASTHUBER, Martin (IT (IT Scientific Computing)); KARNEVSKIY, Mikhail (IT (IT Scientific Computing)); MIDDENDORF, Philipp (FS-CFEL-1 (Forschung mit Photonen Experimente 1)); YAKUBOV, Sergey (IT (IT Scientific Computing)); SCHOOF, Tim (DESY); Dr MARIANI, Valerio (SLAC National Accelerator Lab)

Presenter: Dr WHITE, Thomas (FS-SC)

Session Classification: Poster session and networking lunch

Contribution ID: **4** Type: **Short talk**

RIC and open science

Friday 10 November 2023 10:15 (10 minutes)

Overview of RIC activities for FS, including e.g. results from EU projects and collaborations with LEAPS and Helmholtz.

Primary authors: MILLAR, Alexander Paul (IT (Research and Innovation in Scientific Co)); FUHRMANN, Patrick (IT (Research and Innovation in Scientific Co)); SERVAN, Sophie (DESY); WETZEL, Tim (IT (Research and Innovation in Scientific Co))

Presenter: SERVAN, Sophie (DESY)

Contribution ID: **5** Type: **Short talk**

Borrowing HEP algorithms for detector alignment in photon science

Friday 10 November 2023 11:20 (10 minutes)

Accurate and precise information about the position of the detector is critical to the success of many types of experiment in photon science. This is particularly true for serial crystallography, which is sensitive to detector misalignments of less than one pixel's width. However, serial crystallography data is also very useful for refining the detector geometry, consisting of sharp, bright Bragg peaks in regular and geometrically simple patterns. Several methods have been developed for this process over the last decade. The current state of the art involves refining the "global"detector geometry parameters along with the "local"crystal orientation parameters, in one very large least-squares refinement. The joint refinement of local and global parameters is needed to avoid a biased fit and slow convergence. Unfortunately, with a typical serial crystallography dataset consisting of many tens of thousands of crystals, only a fraction of the data can be used before the refinement becomes too computationally demanding.

The "Millepede"algorithm was developed in high energy physics to address exactly this problem. The relevant matrix equations can be rearranged such that the full calculation can be performed, without approximations but with vastly reduced memory and CPU requirements. This makes a full joint refinement using tens or even hundreds of thousands of crystals practical.

In this contribution, I will describe the ongoing experience of applying the Millepede algorithm to serial crystallography data, and the potential for other applications in photon science.

Primary author: Dr WHITE, Thomas (FS-SC)

Presenter: Dr WHITE, Thomas (FS-SC)

Contribution ID: **6** Type: **Poster**

The imaging program at the SAXSMAT beamline P62

Friday 10 November 2023 13:30 (10 minutes)

Within this contribution, an overview of the imaging program of the SAXSMAT beamline P62 will be given. Especially, the computational aspects of the 3D reconstruction for the SAXS- and WAXS tensor tomography imaging experiments will be presented. Furthermore, an outlook of upcoming projects that include AI in the reconstruction algorithms will be discussed.
Besides the 3D tomography datasets conventional scanning SAXS- and WAXS datasets getting larger and larger and therefore more demanding on the data processing. A short overview of the computational aspects of those data will be discussed as well.

Primary author: Dr HAAS, Sylvio (FS-PETRA-D (FS-PET-D Fachgruppe P62 (SmallAngleSc)))

Presenter: Dr HAAS, Sylvio (FS-PETRA-D (FS-PET-D Fachgruppe P62 (SmallAngleSc)))

Session Classification: Poster session and networking lunch

Contribution ID: **7** Type: **Poster**

Start-to-end Wave Propagation Simulations of Beamlines and Coherence Properties using SRW PIV

Friday 10 November 2023 13:40 (10 minutes)

The FS-PETRA Beamline Optics Simulation group is developing tools and providing support for ray tracing and wave propagation simulations of PETRA beamlines. With the sharp increase of coherence at PETRA IV, wave propagation simulations gain in relevance and will be necessary for many upcoming beamlines. Start-to-end simulations of entire beamlines, including coherent imaging experiments, can be performed.

In my talk I will introduce the principles and simulations of such simulations and explain the unique computing requirements they have.

Primary authors: BAGSCHIK, Kai (DESY FS-PE); SEYRICH, Martin (FS-PETRA (PETRA III)); KHUBBUTDINOV, Ruslan (None)

Session Classification: Poster session and networking lunch

Contribution ID: **8** Type: **Short talk**

Enabling online phase retrieval for in-situ and operando x-ray holography

Friday 10 November 2023 09:45 (15 minutes)

Applying for measurements at large X-ray sources like PETRA III at DESY or BESSY II at HZB is highly competitive. If granted beam time, numerous samples need to be measured. These measurements often occur under in-situ or operando conditions, such as studying the degradation of a biodegradable Mg wire or structural changes in a battery during charging. These changes happen at a sub-micron scale, requiring computationally intensive techniques like phase-sensitive X-ray microscopy. However, these techniques don't provide immediate feedback, increasing the risk of failed measurements and wasted beam time. The Helmholtz imaging project SmartPhase aims to address this issue by providing online reconstruction of measurement data. We are implementing self-optimizing phase-retrieval algorithms based on conventional and physics-informed machine learning approaches.

Primary author: HAGEMANN, Johannes (FS-PETRA (PETRA III))

Co-authors: Mr LOPES, André (Hereon); Dr GREVING, Imke (Hereon (Helmholtz-Zentrum Hereon)); DORA, Johannes (FS-PS (Photon Science)); Dr FLENNER, Silja (Helmholtz-Zentrum Hereon)

Presenter: HAGEMANN, Johannes (FS-PETRA (PETRA III))

Contribution ID: **9** Type: **Short talk**

Modelling the interaction of matter with ultrafast and ultraintense x-ray pulses

Friday 10 November 2023 10:00 (15 minutes)

I present an overview over the simulation activities done with the XRAYPAC tookit developed at FS-CFEL-3.

Primary authors: Dr INHESTER, Ludger (CFEL, DESY); SON, Sang-Kil (FS-CFEL-3 (FS-CFEL-3 Fachgruppe 3)); JUREK, Zoltan (FS-CFEL-3 (Forschung mit Photonen Theorie))

Presenter: Dr INHESTER, Ludger (CFEL, DESY)

Contribution ID: **10** Type: **Poster**

Beamline P11

Friday 10 November 2023 13:20 (10 minutes)

We'll give an overview of our computational projects at beamline P11.

Primary authors: Dr GRUZINOV, Andrey (DESY); POMPIDOR, Guillaume (DESY); HAKANPAEAE, Johanna (FS-PETRA-D (FS-PET-D Fachgruppe P11))

Co-authors: TABERMAN, Helena (FS-PETRA-D (FS-PET-D Fachgruppe P11)); MERKULOVA, Olga (IK Company); POTTURU, Sreenivasula Naidu (CMS (CMS Fachgruppe DAQ, SW, Computing))

Session Classification: Poster session and networking lunch

Contribution ID: **11** Type: **Short talk**

FS-EC: Software solutions in the critical path for data acquisition

Friday 10 November 2023 09:15 (10 minutes)

Within FS-EC (Experiment Control) we develop and adopt software solutions that cater the data acquisition processes in user operation in FS facilities as well as fundamental background services that are needed for a performant beamline infrastructure. The group covers aspects spanning across high level controls (Sardana), low level controls and hardware abstraction (Tango), detector drivers and adaptors (for high speed cameras), custom firmware for embedded devices (PILC) to beamline specific scripts and user interfaces. Further we are involved in data analysis (Maxwell support) as well as GPFS storage (ASAP3) related activities.
As one of the support groups within FS our mission is to contribute to smooth user operation in DESY FS facilities. This involves own developments (e.g. hundreds of Tango servers) as well as the contributions to international collaborations.

Primary author: PITHAN, Linus (FS-EC (Experimente Control))

Presenter: PITHAN, Linus (FS-EC (Experimente Control))

Contribution ID: **12** Type: **Short talk**

Overview of central IT for FS

Friday 10 November 2023 10:25 (10 minutes)

A short overview of the services provided by central IT specifically for FS data taking and data processing, especially the ASAP3 framework and related services.

Primary author: HANNAPPEL, Juergen (IT (IT Scientific Computing))

Presenter: HANNAPPEL, Juergen (IT (IT Scientific Computing))

Contribution ID: **13** Type: **Short talk**

Welcome and introduction

Friday 10 November 2023 09:00 (10 minutes)

Presenters: WECKERT, Edgar (FS (Forschung mit Synchrotronstrahlung)); BARTY, Anton (FS-SC (Scientific computing))

Contribution ID: **14** Type: **Short talk**

Martin Burger - FS-CI

Friday 10 November 2023 09:25 (10 minutes)

Presenter: BURGER, Martin (FS-CI (Computational Imaging))

Contribution ID: **16** Type: **Short talk**

Philipp Neumann - Central IT

Friday 10 November 2023 09:10 (5 minutes)

Presenter: NEUMANN, Philipp (IT (Informationstechnik))

Contribution ID: **18** Type: **Short talk**

The AMARCORD electronic log book

Friday 10 November 2023 13:35 (15 minutes)

Presenter: MIDDENDORF, Philipp (FS-CFEL-1 (Forschung mit Photonen Experimente 1))

Session Classification: Poster session and networking lunch

Contribution ID: **20** Type: **Short talk**

X-Environment metadata management

Friday 10 November 2023 12:00 (15 minutes)

Presenter: KHOKHRIAKOV, Igor (FS-SC (Scientific computing))

Contribution ID: **21** Type: **not specified**

Protein Machinists: Teasing out the secrets of subtle protein dynamics

Friday 10 November 2023 09:35 (10 minutes)

The knowledge gap between what we know about proteins and what we would like to do with them is broadly described as "protein dynamics". The nascent Protein Machinists group tackles this from computational angles: how to mathematically express protein conformations, compare them, establish what is contained within an experimentally observed population and manipulate them. I will also talk about the computational backbone of the scientific work.

Presenter: Dr GINN, Helen (DESY-FS)

Contribution ID: **22** Type: **Short talk**

Real-time data processing for serial crystallography at P11

Friday 10 November 2023 11:05 (15 minutes)

Presenters: SCHOOF, Tim (DESY); Dr WHITE, Thomas (FS-SC)

Contribution ID: **23** Type: **Short talk**

Data processing and management at P06

Friday 10 November 2023 12:15 (15 minutes)

Presenter: GARREVOET, Jan (FS-PETRA-S (FS-PET-S Fachgruppe P06))

Contribution ID: **25** Type: **Poster**

DAPHNE4NFDI

Friday 10 November 2023 12:40 (5 minutes)

Presenter: BARTY, Anton (FS-SC (Scientific computing))

Session Classification: Poster session and networking lunch

Contribution ID: **26** Type: **not specified**

RockIT project

Presenter: Dr SCHOEKEL, Alexander (DESY)

Contribution ID: **27** Type: **Poster**

DASHH

Friday 10 November 2023 12:45 (5 minutes)

Session Classification: Poster session and networking lunch

Contribution ID: **44** Type: **not specified**

Enabling online phase retrieval for in-situ and operando x-ray holography

Presenter: HAGEMANN, Johannes (FS-PETRA (PETRA III))

Contribution ID: **45** Type: **not specified**

Modelling the interaction of matter with ultrafast and ultraintense x-ray pulses

Presenter: SON, Sang-Kil (FS-CFEL-3 (FS-CFEL-3 Fachgruppe 3))

Contribution ID: **47** Type: **Poster**

RockIT project

Friday 10 November 2023 12:50 (15 minutes)

Presenter: Dr SCHOEKEL, Alexander (DESY)

Session Classification: Poster session and networking lunch

Contribution ID: **48** Type: **Poster**

Shaking out Intrinsic Structural Variation in Femtosecond Protein Crystallography using Deep Learning

Friday 10 November 2023 12:35 (5 minutes)

Current femtosecond crystallography data processing routines such as CrystFEL by T. White generally assume that identical molecular structure for each of the tens of thousands of protein crystals used. This assumption is however known to be unphysical, and with the recent development of deep learning technology, we are exploring whether we can build a net capable of shaking out the subtle structural variation information hidden behind a cloud of noise. We report progress on the development of a variational autoencoder, with an architecture inspired both from work in particle physics and Cryo EM.

Primary authors: JAKOBSEN, Mads Bregenholt (FS-SC (Scientific computing)); FLEWETT, Samuel (FS-SC (Scientific computing)); Dr WHITE, Thomas (FS-SC)

Presenter: FLEWETT, Samuel (FS-SC (Scientific computing))

Session Classification: Poster session and networking lunch

Contribution ID: **49** Type: **Short talk**

Data Handling and Analysis at FLASH

Friday 10 November 2023 11:30 (15 minutes)

This presentation offers a succinct examination of FLASH, emphasizing the facility's key features. It outlines the IT infrastructure and collaborative relationships with different DESY groups. Additionally, it delves into the technical aspects of experimental control, data acquisition, and analysis methods. The talk also sheds light on current projects and future directions.

Primary author: PASSOW, Christopher (FS-FLASH-D (FLASH Photon Diagnostics and Controls))

Presenter: PASSOW, Christopher (FS-FLASH-D (FLASH Photon Diagnostics and Controls))

Contribution ID: **51** Type: **Poster**

Computational Imaging @ DESY

Friday 10 November 2023 13:05 (5 minutes)

We will present the work and expertise of the newly established Computational Imaging Group at DESY. Being founded in mathematics, we provide expertise in inverse problems as well as theoretical foundations of machine learning methods.
We give an overview of mathematical methods in imaging and applications thereof, in particular algorithms for reducing computational cost in large scale problems. Moreover, we give insight into theoretically founded training of robust or sparse neural networks.

Primary authors: ROITH, Tim (FS-CI (Computational Imaging)); BURGER, Martin (FS-CI (Computational Imaging)); KUGER, Lorenz (FS-PS (Photon Science)); Ms KABRI, Samira (FS-CI (Computational Imaging)); WEIGAND, Lukas (FS-CI)

Presenter: ROITH, Tim (FS-CI (Computational Imaging))

Session Classification: Poster session and networking lunch

Contribution ID: **52** Type: **Poster**

Molecular states for quantum simulation

Friday 10 November 2023 13:10 (10 minutes)

Can laser-induced molecular wave packets be used as a quantum simulator?

Primary author: TRIPPEL, Sebastian (FS-CFEL-CMI (CFEL-CMI Controlled Molecule Imaging))

Presenter: TRIPPEL, Sebastian (FS-CFEL-CMI (CFEL-CMI Controlled Molecule Imaging))

Session Classification: Poster session and networking lunch