Research Field Structure of Matter: Programme PNI

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The High Data Rate Initiative (HDRI) of the Helmholtz Program 'Photon, Neutron and Ions' (PNI)

Edgar Weckert
DESY

Layout

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- Introduction to PNI
- Data rates at PNI facilities
- Structure and aims of HDRI
- Status of HDRI and possible connections to LSDMA
- Summary and Outlook

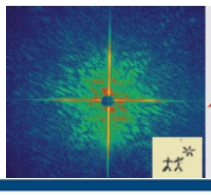
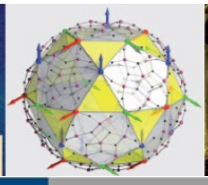
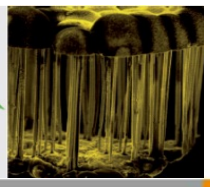
Introduction: PNI Mission

Photons, neutrons and ions are complementary probes for research ranging from condensed matter to molecules, atoms and plasmas

The programme PNI operates and constructs large scale facilities providing photons, neutrons, and ions of often unsurpassed quality or quantity

PNI focusses on providing external users with first rate research opportunities and specialized expert support

PNI pursues a vigorous in-house research programme in basic and applied science

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DESY
KIT Karlsruhe Institute of Technology
GKSS Forschungszentrum
GSI
HZB Helmholtz Zentrum Berlin
FZD Forschungszentrum Dresden Rossendorf

Introduction: PNI Photon Sources

FLASH

BESSY II

ANKA

European XFEL

PETRA III

DORIS III

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Introduction: PNI Neutron Sources/Activities

Guide Hall
BER-2 / HMI

Guide Hall
FRM II / FZJ,GKSS, HZB outstations

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Jülich Centre for Neutron Science

HZB Helmholtz Zentrum Berlin

GKSS FORSCHUNGSZENTRUM

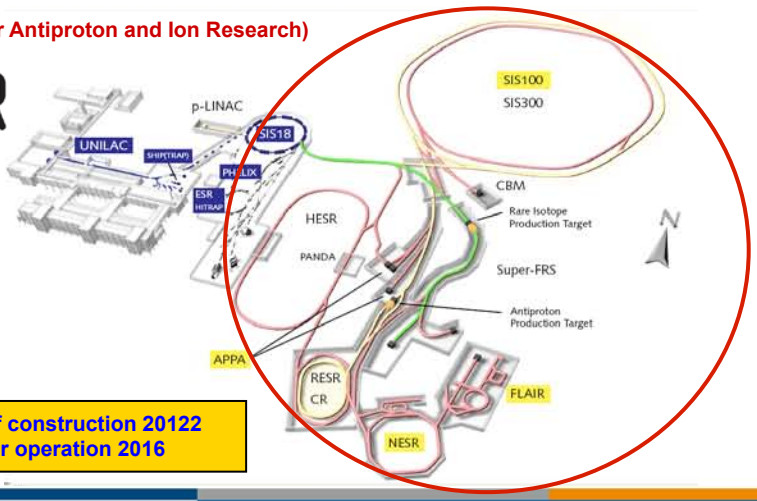
First Intl. LSDMA Symposium

Introduction: PNI Ion Sources

CN DE ES FI FR GB GR IN IT PL RO RU SE

(Facility for Antiproton and Ion Research)

FAIR



Start of construction 20122
user operation 2016

First Intl. LSDMA Symposium

Motivation for HDRI

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Present situation:

- new high brilliance synchrotron radiation, free electron laser, neutron and ion sources (have) starting operation (PETRA III, SNS, FLASH, …, XFEL, FAIR)
- large efforts are made for more efficient detection scheme like extremely fast 2D pixel detectors
- experiments deliver extremely high peak and average data rates (O(100 GB/h))
- data rates are expected to increase in future
- experimentalists have only in rare cases a possibility for a real-time data analysis for e.g. quality check, visualisation and evaluation
- handling of these amounts of data poses a heavy burden on users as well as on facility staff
- various PNI centers have special expertise and requirements for specific experiments carried out at their facilities

Examples for High Data Rate Detectors

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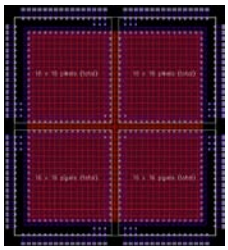
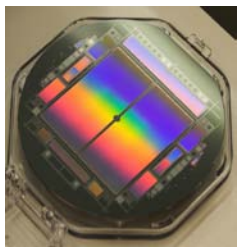
4k x 4k pixels
1 s readout
16 MB/s
56 GB/h
DS: 10 GB

Pilatus
6 M pixels
12 Hz frame rate
180 MB/s
630 GB/h
DS: 10 - 30 GB



APD array
32 x 32 pixels
300 microns
~ 1 nsec timing
few nsec framing
24 GB/s !
➔ Hardware correlator needed
DS: 2 MB



pnCCD
1k x 1k pixels
250 Hz frame rate
500 MB/s
1.7 TB/h
DS: 20 TB (e.g. one week at LCLS)

XFEL detectors under development: 1 M pixels x 400 frames x 10Hz ➔ 7.8 GB/s (maximum)

Superconducting pulsed RF bunch structure

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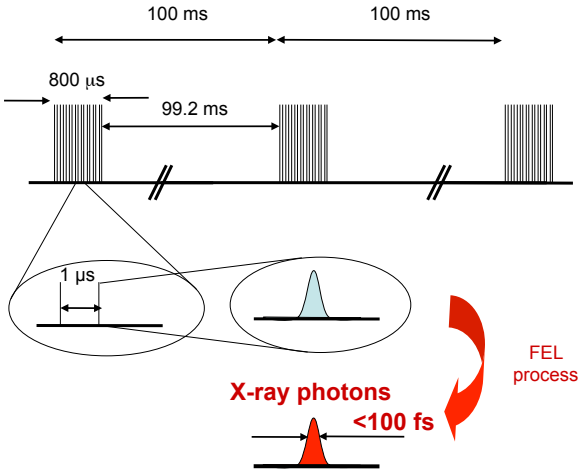

- up to 27000 bunches per second
- very high intensities (up to 10^{13} ph/bunch)
- high repetition rates (up to 4.5 MHz)
- large variability
  - pulse patterns
  - pulse to pulse variations

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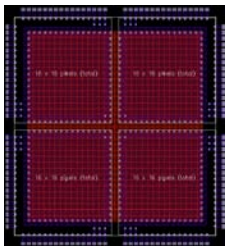

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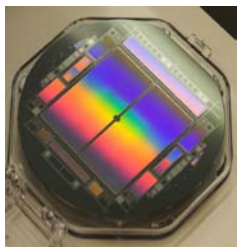

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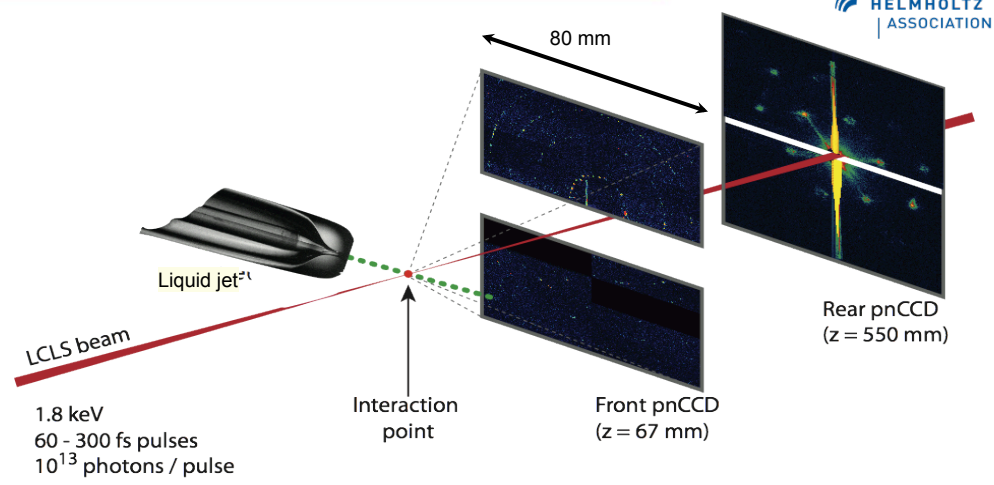
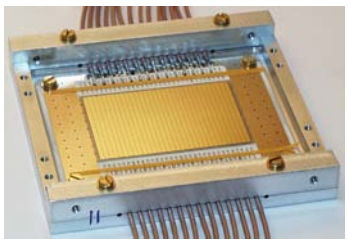
Nanocrystallography carried out in a flowing water microjet



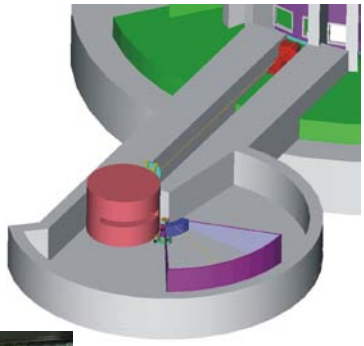
Chapman, Barty (CFEL/DESY), Spence, Fromme (ASU), Hajdu (U. Uppsala), et al.

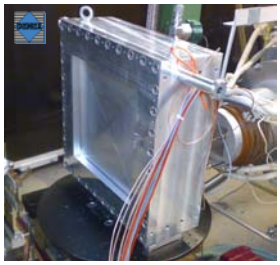
Examples for High Data Rate Detectors



32 diamond-strip
heavy ion detector
4 TB/h
DS: 2-4 GB/h

DENS (planned)
200Mb/Pulse ➔12 Gbyte/sec
DS: 4TB/h





^{3}He DENEX
detector
10 MB/s
36 GB/h
DS: 2 GB/d

Requirements

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What is needed:

- **an efficient use of the available beamtime demands for**
  - **an almost real-time evaluation of the measured data**
  - **sufficient information on whether the data collection process was successful**
- **this requires fast:**
  - **first data reduction**
  - **computation of data quality indicators or**
  - **reconstruction and/or**
  - **visualization**
  - **modeling**
- **this data handling needs to be fast enough to guide the experiment**
- **complete data lifetime management**
  - **data collection including all relevant meta data**
  - **fast first reduction and evaluation**
  - **final evaluation/reconstruction**
  - **(remote) user access**
  - **long term archiving**

Definitions

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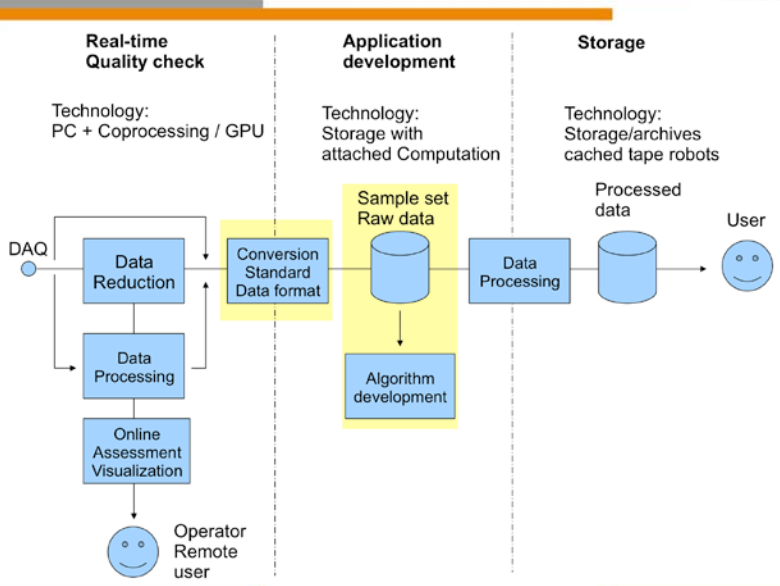

Scope of the Proposed Activities

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Aims of this Initiative (I):

- join forces and expertise within PNI for a common effort
- avoid duplications of effort
- create a platform for common development of data evaluation strategies and software (PNI-centers, other facilities and user community)
- establish standardized data formats for easy exchange of evaluation software
  - requires also an agreement on the appropriate amount of meta-data and information saved for each experiment
  - adopt standards established elsewhere
- develop/implement/adapt soft- and hardware solutions:
  - to enable fast real time data evaluation → first results within ~minutes
  - to enable real-time reconstruction or visualization where needed
  - to facilitate handling, access and archiving large amounts of data
- establish a framework for modeling and simulation of experimental data
  - highly automated and user friendly evaluation software

Scope of the Proposed Activities

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Aims of this Initiative (II):

- focus during the first years on those developments needed most urgently by the user community
  - (protein) crystallography
  - µ-tomography, (hard X-ray) imaging
  - [A,GI,U][W,S]A[X,N]S
  - correlation spectroscopy, fluorescence mapping
  - [p,n,I]-TOF – spectroscopy
  - ion charge state spectroscopy
- use the developed soft- and hardware building blocks for the implementation of further experimental techniques
- extend this initiative beyond the current five year PoF-period
- collaborate with non-PNI partners as close as possible

Coordination

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Organization in three major work packages:

1. Data management (coordinated by DESY, HZB)
2. Real Time Data Processing (coordinated by KIT, GSI)
3. Data analysis, modeling and simulation (coordinated by FZJ)

Structure of the initiative:

- **HDRI Steering Committee (HDRI-SC)**
  - program speaker and topic speakers
  - additional member of each PNI center if not already represented
  - coordinators of the work packages
  - chair person and managing coordinator will be nominated
  - meets twice a year
  - decides on strategic directions of the initiative
- **Managing Coordinator (Rainer Gehrke, DESY)**
  - coordination tasks within HDRI
  - coordinates the collaboration between centers and non-PNI members
- **HDRI General Assembly (HDRI GA)**
  - all persons involved in HDRI
  - meets once a year
  - discusses status and activities

Dissemination/Communication

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Exchange of information and software:

- **HDRI Web Page** (http://www.pni-hdri.de)
  - news
  - event calendar
  - workshop announcement
  - defined standards
  - documentation (e.g. wiki)
  - software download
- **HDRI workshops**
  - dedicated to specific topics
  - discussion of work package contents, status and objectives
  - invite external experts and collaborators
  - hands on courses for non experts

Collaboration with non-PNI partners:

- **Visualization of SAS and WAS data**
- **VEDAC, PANdata, NMI3 data analysis working group**
- **Questions to be considered: (i) IP-issues, (ii) existing standards**

Status of HDRI / Connection to LSDMA

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- **WP1:**
  - The basic definition of a standardized data format is available (based on NeXuS/HDF5).
  - A programming interface has been created. It is public available and serves data acquisition software to write data compliant to the standard.
  - Implementation at various beamlines is ongoing (DESY).
  - Further enhancements of HDF5 are planned together with HDF5 development group to allow third party data suppliers to implement additional functionality (filters).
  - Data archiving will be based on dCache (DESY, FermiLab)
  - A data portal for users is in preparation. This includes a worldwide common authentication system, remote data access and processing, and a searchable catalogue for meta data.

Status of HDRI / Connection to LSDMA

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- **WP2:**
  - The potential of accelerating data processing by means of state-of-the-art computing hardware was extensively studied.
  - A first demonstrator for very fast µ-tomographic reconstruction has been successfully created (KIT, GPU based, hard- and software).
  - An application in the field of Small Angle Scattering is currently under investigation.
- **WP3:**
  - A framework for real time data processing has been created and first data evaluation workflows have been implemented for specific experimental techniques (already in practical use).

Conclusion and Outlook

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HDRI is an unique opportunity for:

- **a major improvement of fast online data handling, visualisation and analysis at PNI facilities for all users**
- **most efficient use of the available beamtime**
- **make expert evaluation programs available to non expert users**
- **common enterprise of all PNI centers**
- **open for collaborations of all kind**
- **strategic long term (> 5 years) collaboration for development of critical software**
- **long term goal: electronic gateway for the access of all experimental data as well as the necessary evaluation software**

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Thank you for your attention