New opportunities in Photon Science with high-speed X-ray imaging detector CITIUS, and associated data challenge

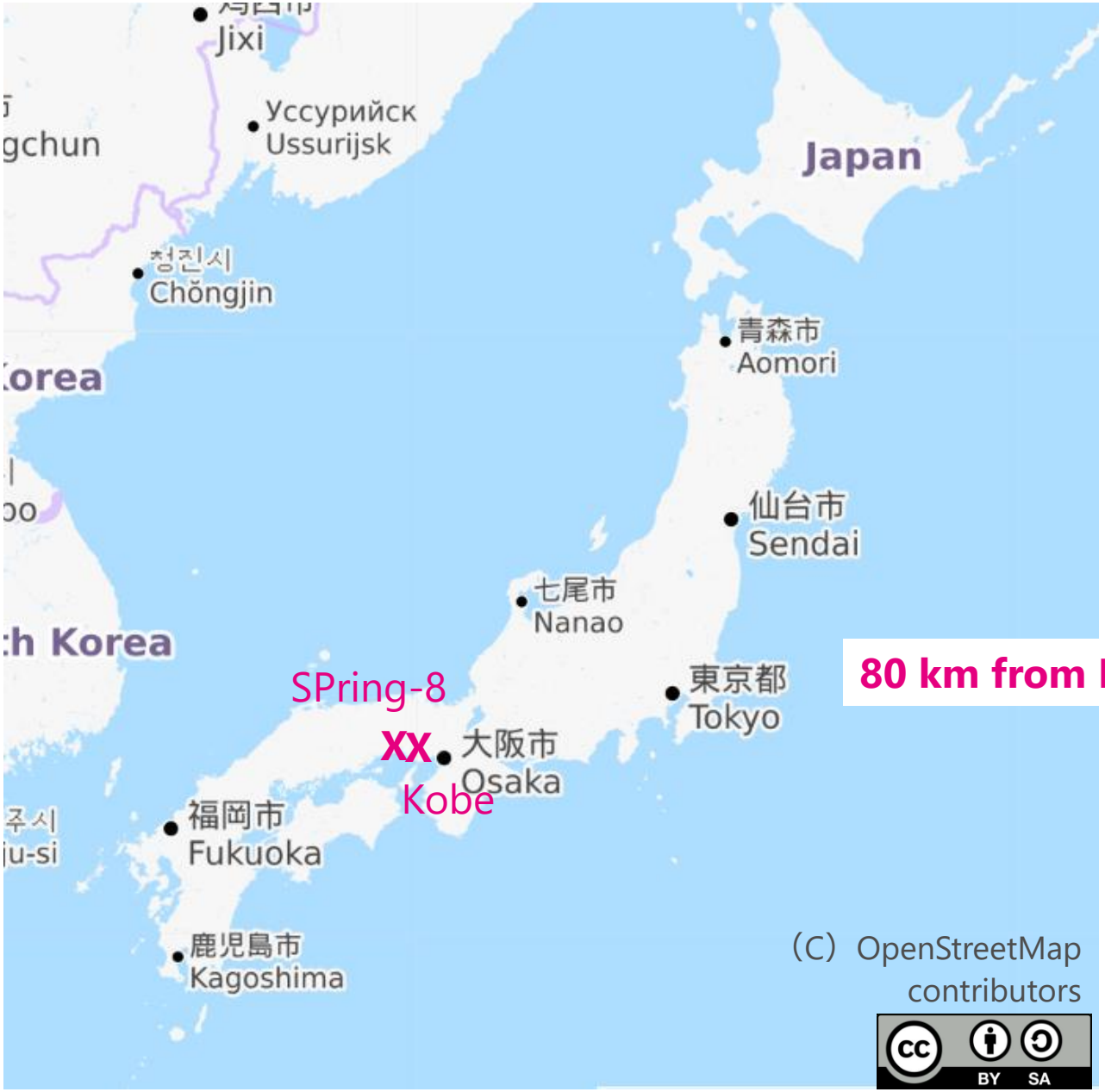
Takaki Hatsui

RIKEN SPring-8 Center

Outline

- Photon science in 2020s
- Detector Technology: New Trends
  - CITIUS detector
- Data Challenge
- Summary

Where ?


Jixi
Уссурийск
Ussurijsk
gchun
Japan
청진시
Chŏngjin
青森市
Aomori
Korea
仙台市
Sendai
七尾市
Nanao
h Korea
SPring-8
東京都
Tokyo
XX
大阪市
Osaka
Kobe
福岡市
Fukuoka
주시
ju-si
鹿児島市
Kagoshima
80 km from R-CCS
(C) OpenStreetMap contributors
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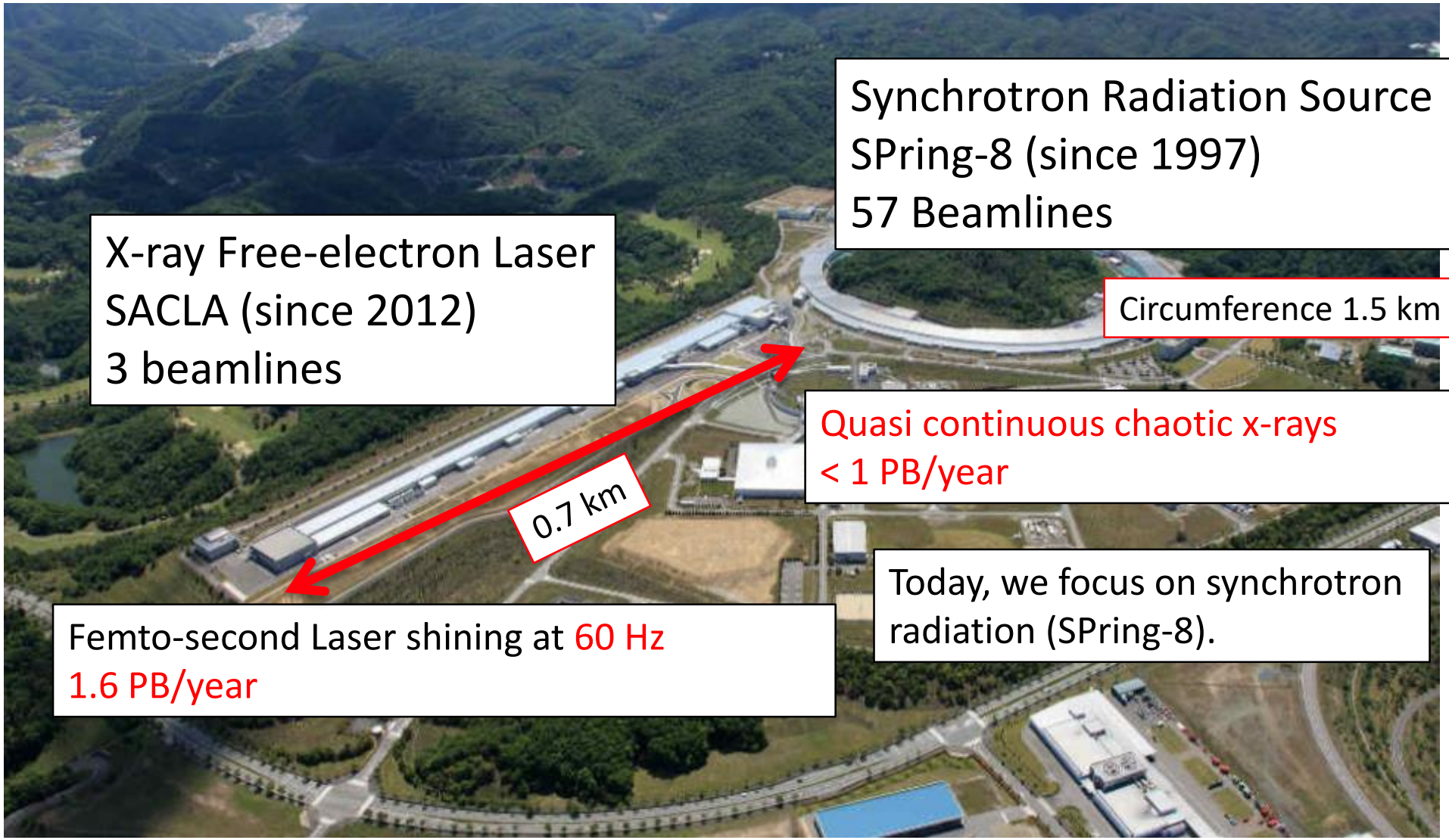
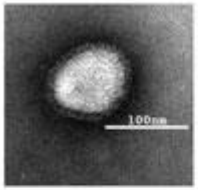
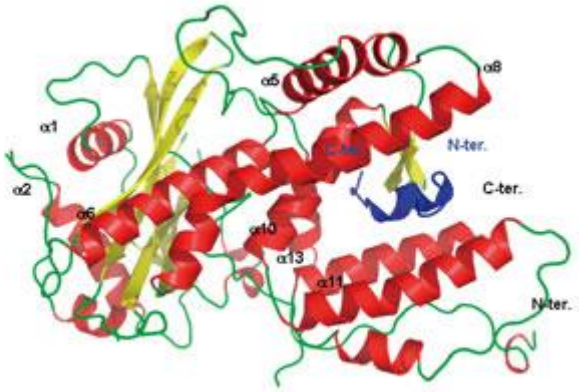
Photon Science: X-ray Science based on Accelerators
SPring-8 Site



SPring-8 Science Highlights (from MEXT web site)

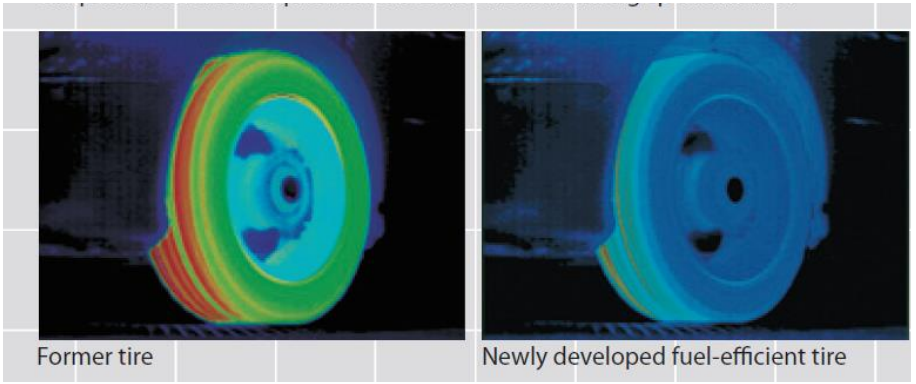
- Macromolecule structure





In July 2008, Dr. Sam-Yong Park of Yokohama City University clarified the structure of an important section of a protein related to influenza virus, which will lead to the development of new drugs.

- Polymer science

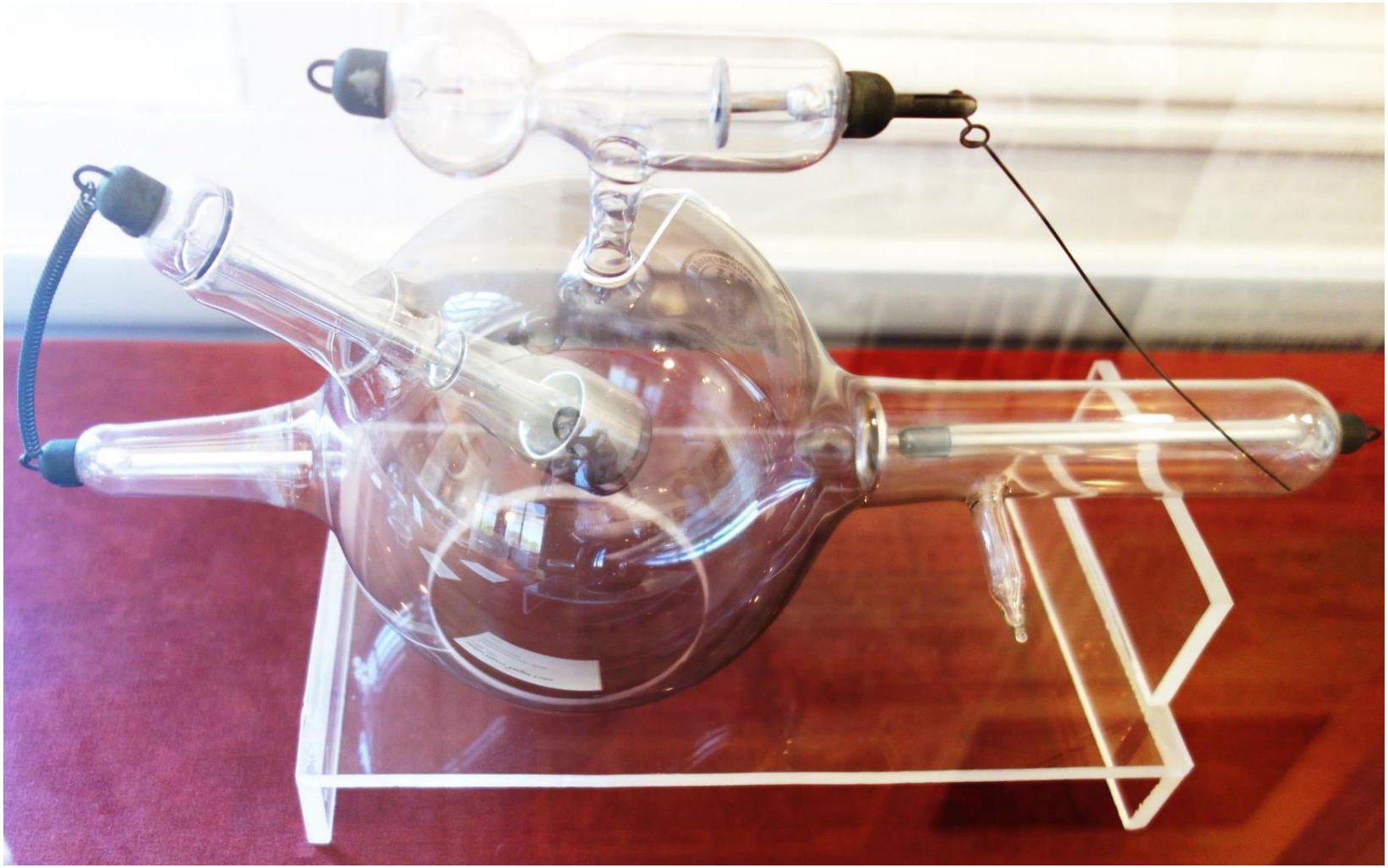


Development of high performance, fuel-efficient tires was enabled by utilizing SPring-8, J-PARC, and K computer

More can be found at SPring-8 web site
http://www.spring8.or.jp/en/news_publications/research_highlights/

How to generate X-rays?

Müuller Heavy Target Tube ca 1890-1910



Museum Dedicated to Surgical Science, Chicago

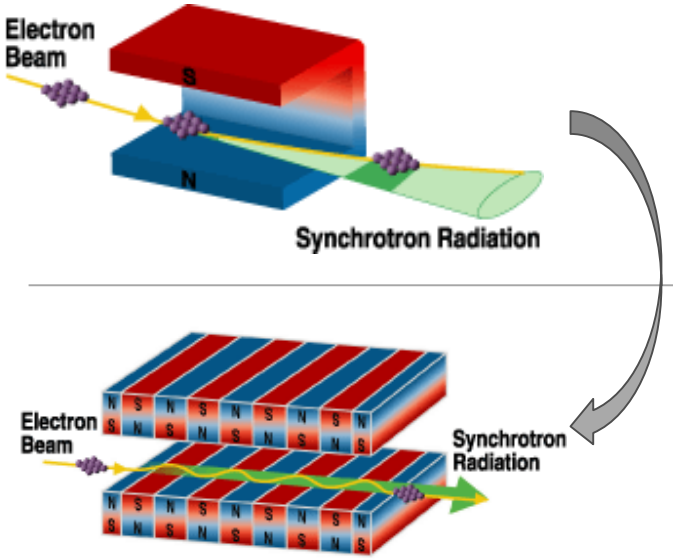
X-ray Tube, Synchrotron Radiation

electron

Atomic Nuclei

Brilliance (photons/sec/mm^2/mrad^2/0.1% B.W.)

ca. 1990	10^7
ca. 1960s	10^8
Late 70's/early 70's	10^{12}
1982: Photon Factory	10^{17}
1994: ESRF 1996: APS 1997: SPring-8 2013: Petra III	$10^{19\text{-}21}$



$(N_{magnet})^1$

$(N_{magnet})^2$

Moore's Law 2x in 18 months

Synchrotron Radiation brightness 3x in 18 months

Shpyrko O G 2004 Experimental x-ray studies of liquid surfaces PhD Thesis Harvard University

X-ray Tube, Synchrotron Radiation

electron

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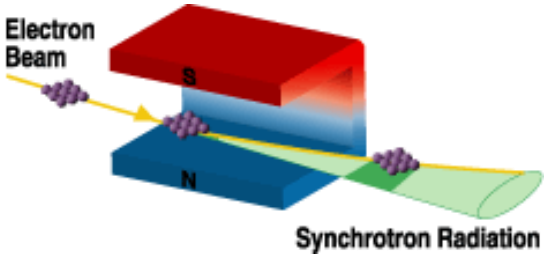

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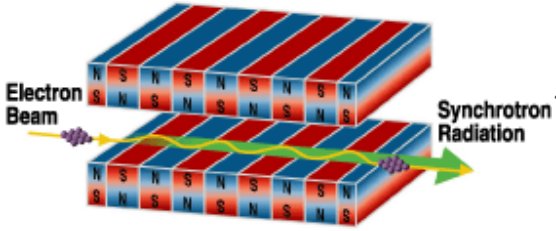


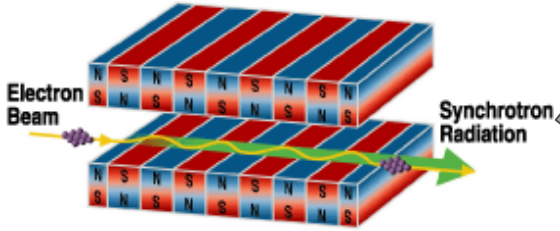
1994: ESRF

1996: APS

1997: SPring-8

2007: Petra III

$10^{19\text{-}21}$



Multi-bend achromat electron lattice

2020: ESRF EBS

2024: APS-U

202X: Petra IV

202X: SPring-8-II

$10^{22\text{-}23}$

Outline

- Photon science in 2020s
- **Detector Technology: New Trends**
  - **CITIUS detector**
- Data Challenge
- Summary

X-ray Material Interactions
X-ray Imaging detector needs

Fluorescence

$I_F \propto A$

X-ray photon energy detection

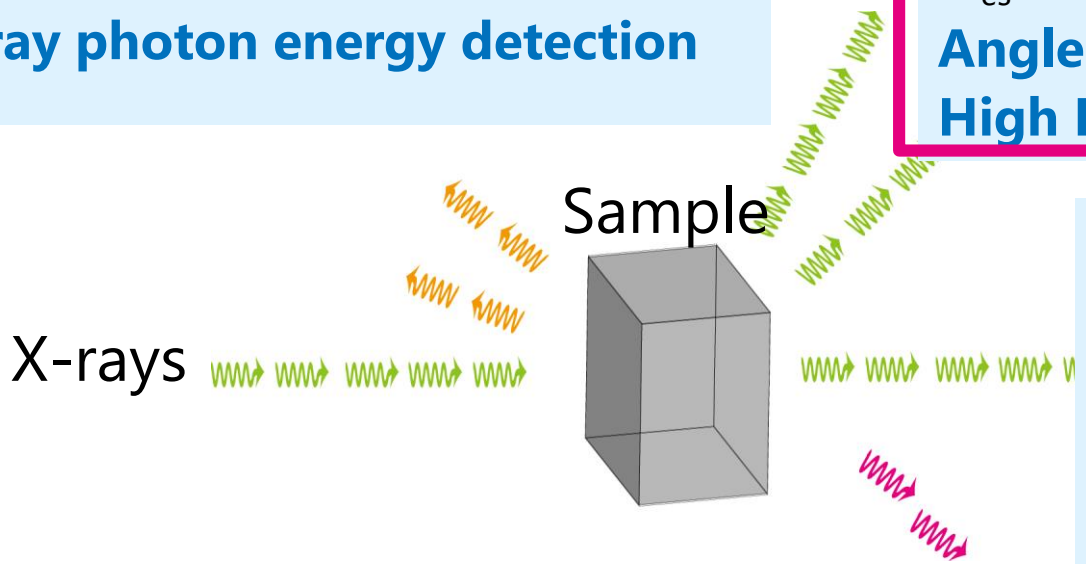
Elastic scattering/diffraction

$I_{es} \propto q^{-4}$ *(uniform material)*

$I_{es} \propto E_{ph}^{-2}$

Angle detection: ~sub 100 µm pixel

High Dynamic Range Imager



Absorption

$A = -\log(I/I_o)$

Focused Image: high spatial resolution sub 1 µm

High dynamic range imager

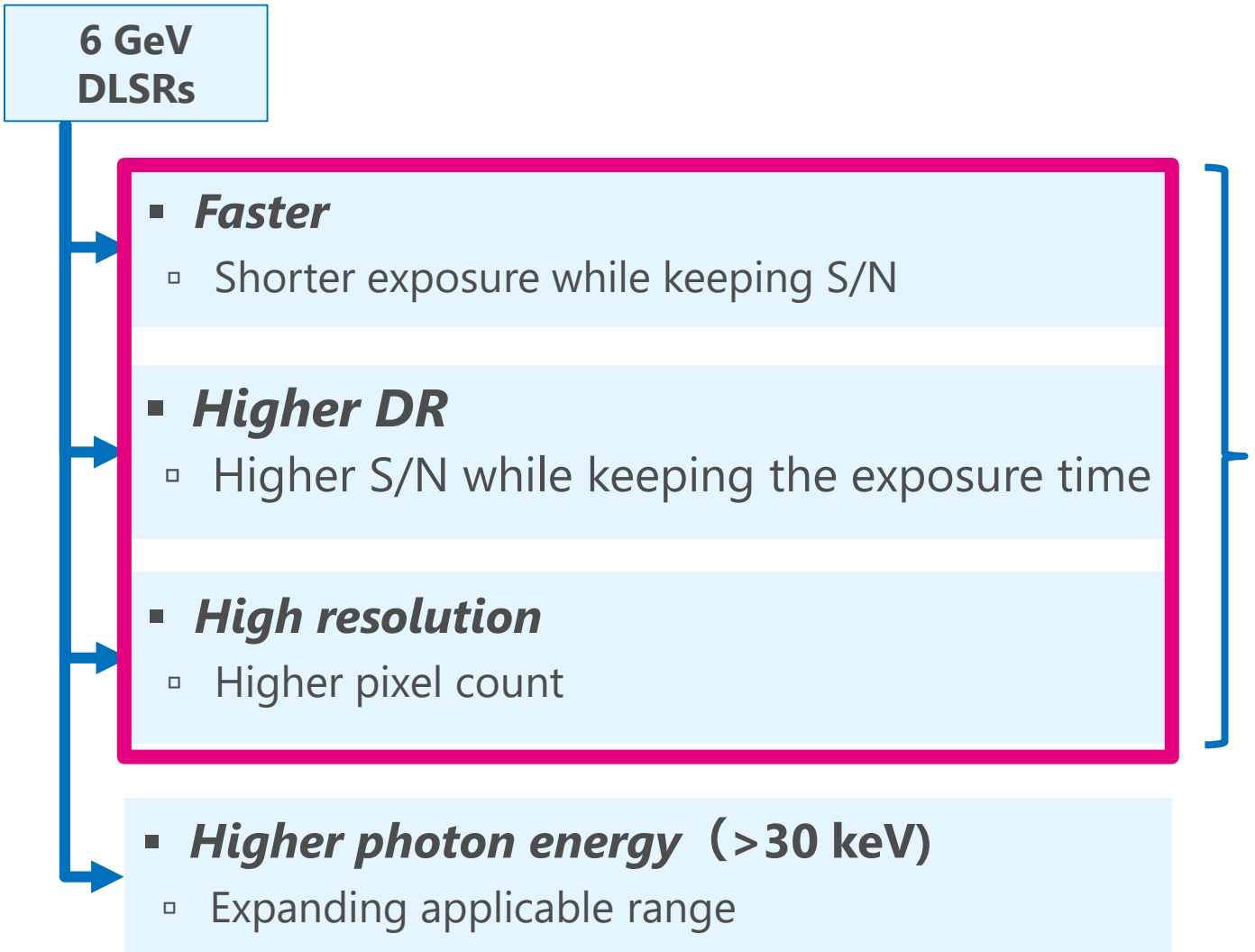
Inelastic scattering (Compton, nuclear resonance,,,)

X-ray photon energy detection

Vector detection

arrival time detection

Introduction: What is needed toward SPring-8-II



- Achieve these **simultaneously** while keeping the beauty of the existing detectors.

CITIUS detector

(Charge Integration Type Imaging Unit with high-Speed extended-Dynamic-Range Detector)

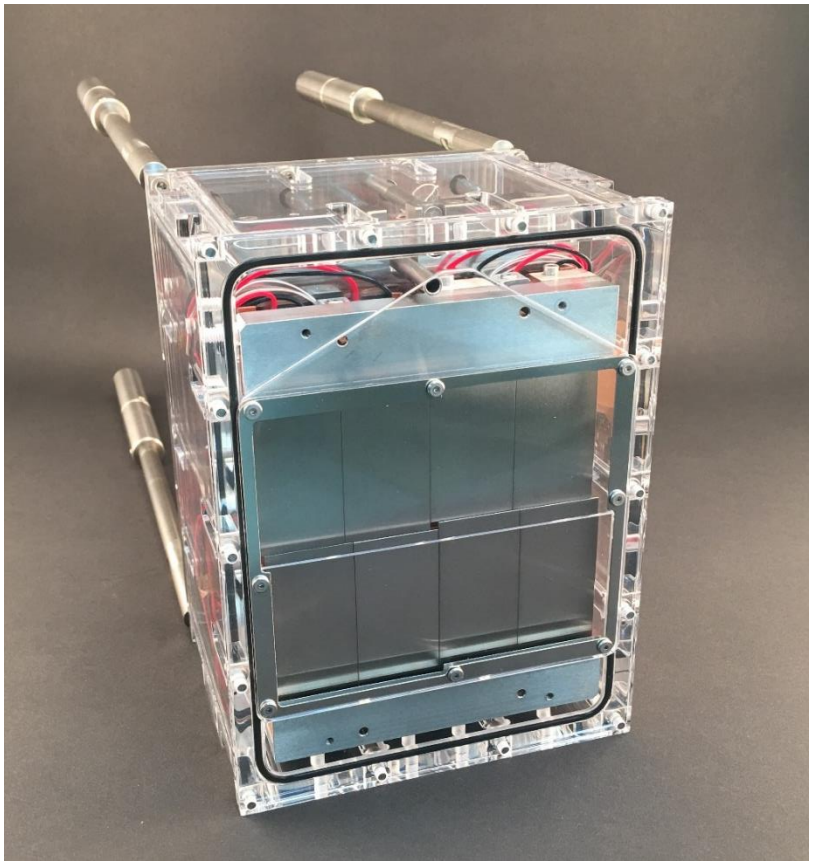
Main Project Target
for scattering/diffraction experiments

CITIUS Detector Development 2013-2020

2.28 Mpixel Camera Head (Mock-up)

Sensor Module	Pixel Size	72.6 μm
	Pixel number	0.28 Mpixel/sensor
	Peak Signal	1800 phs.@12 keV
	Noise	0.02 phs.@12 keV
	Frame Rate	17.4 kHz
	Saturation Count rate	30 (600) Mcps

Detector System	Pixel Number	Max. 20 Mpixel
	Imagine area	Max. 32 x 32 cm^2



Tiling Sensor Modules: Parallel in nature

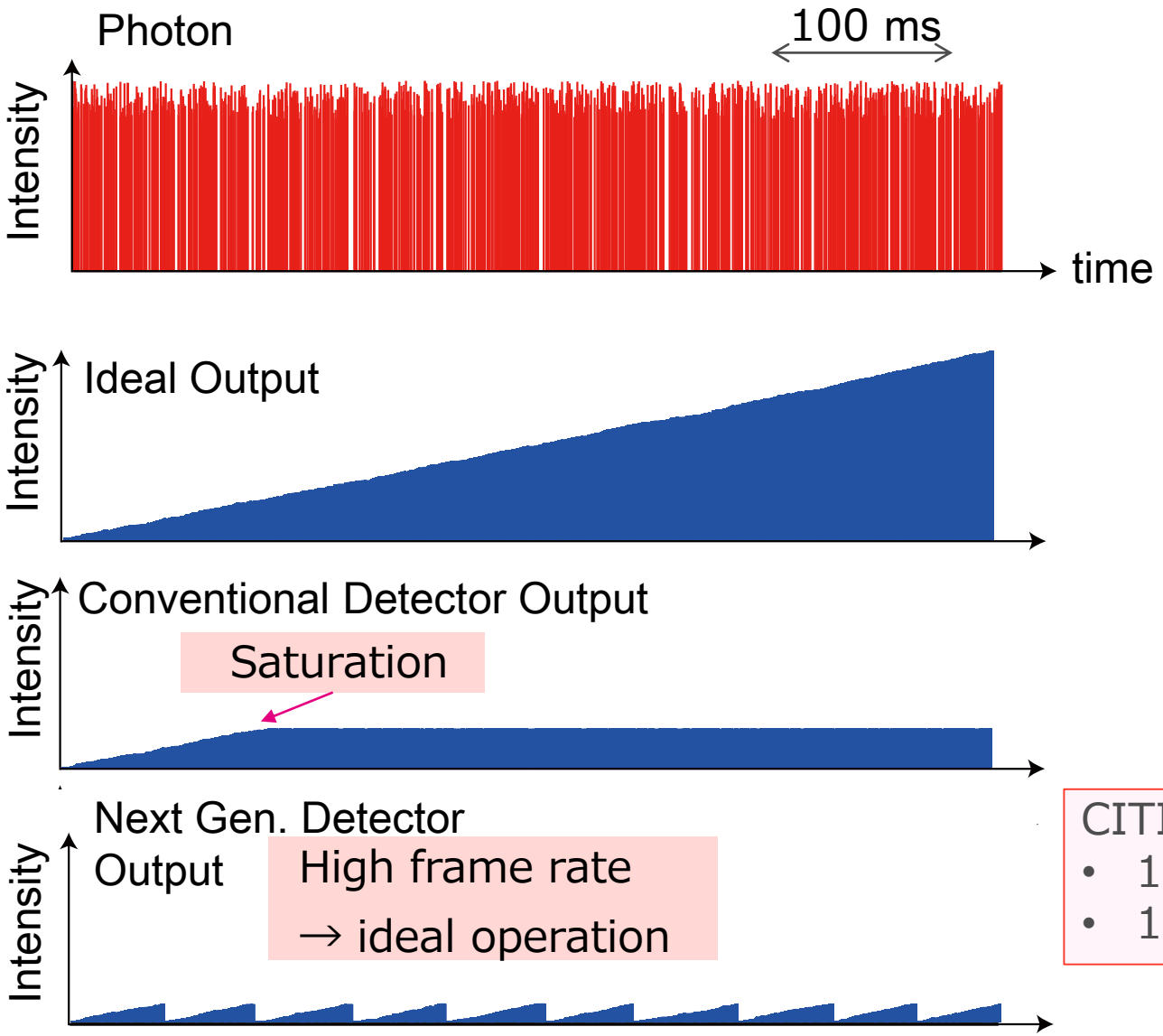
CITIUS Prototype Camera

K. Ozaki, Y. Honjo,
T. Kudo, T. Hatsui

Prototype sensor

- Produced in 2018
- 70 kpixels
- Capacitive and resistive load to mimic final 0.28 Mpixels
- Data output of 0.28 Mpixels with dummy pixels

High Dynamic Range



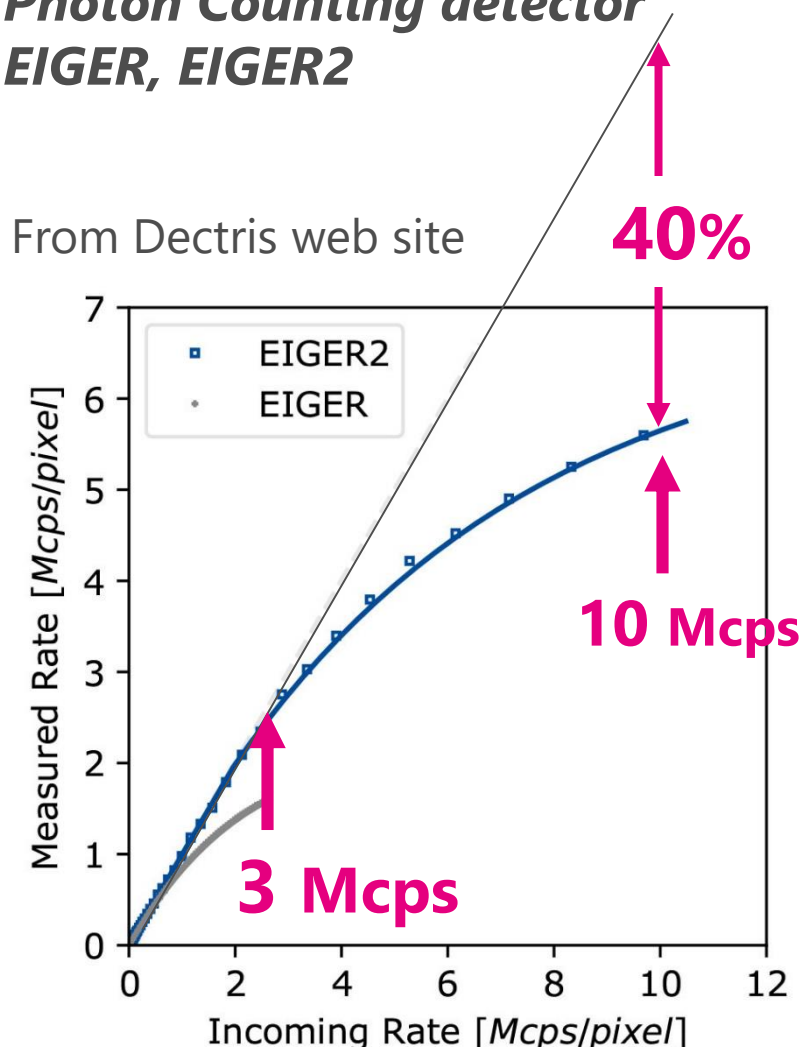
CITIUS detector
- 17.4 kfps
- 1800 photons/frame

Count Rate

K. Ozaki, Y. Honjo, T. Hatsui

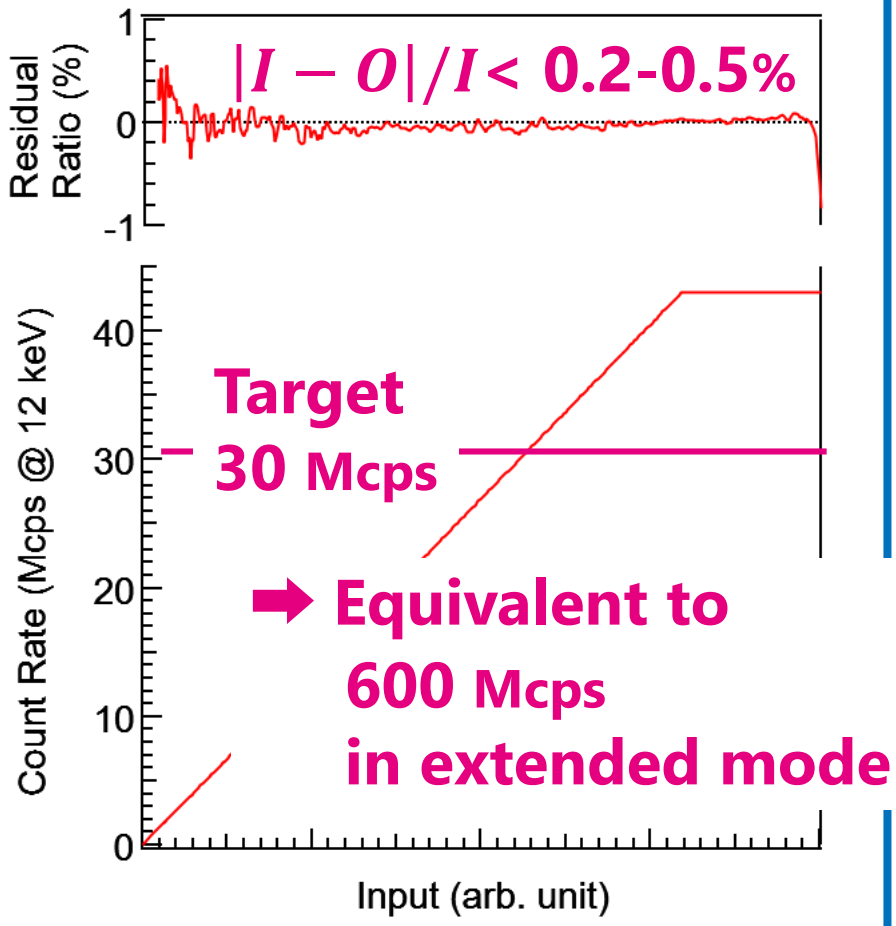
Conventional
Photon Counting detector
EIGER, EIGER2

From Dectris web site



Next Generation
Charge Integrating detector
CITIUS

Measurement with Proto camera

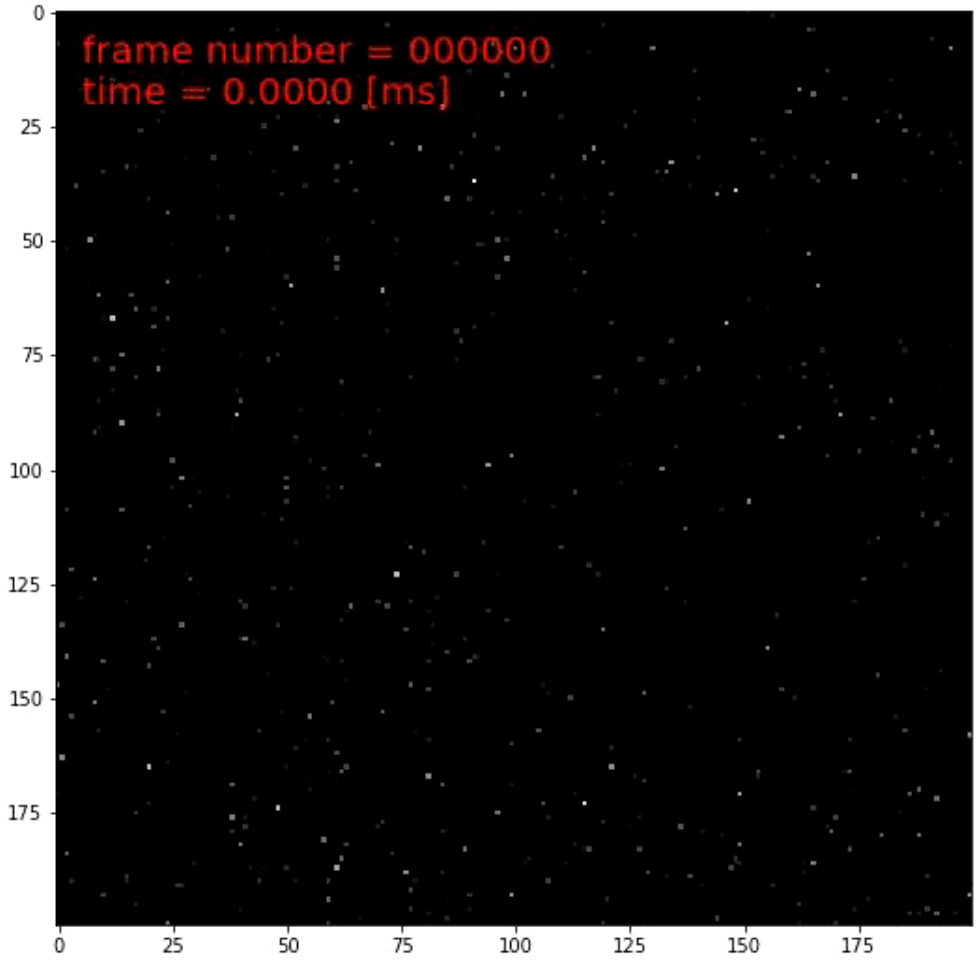


Transmission Image@17.4 kfps

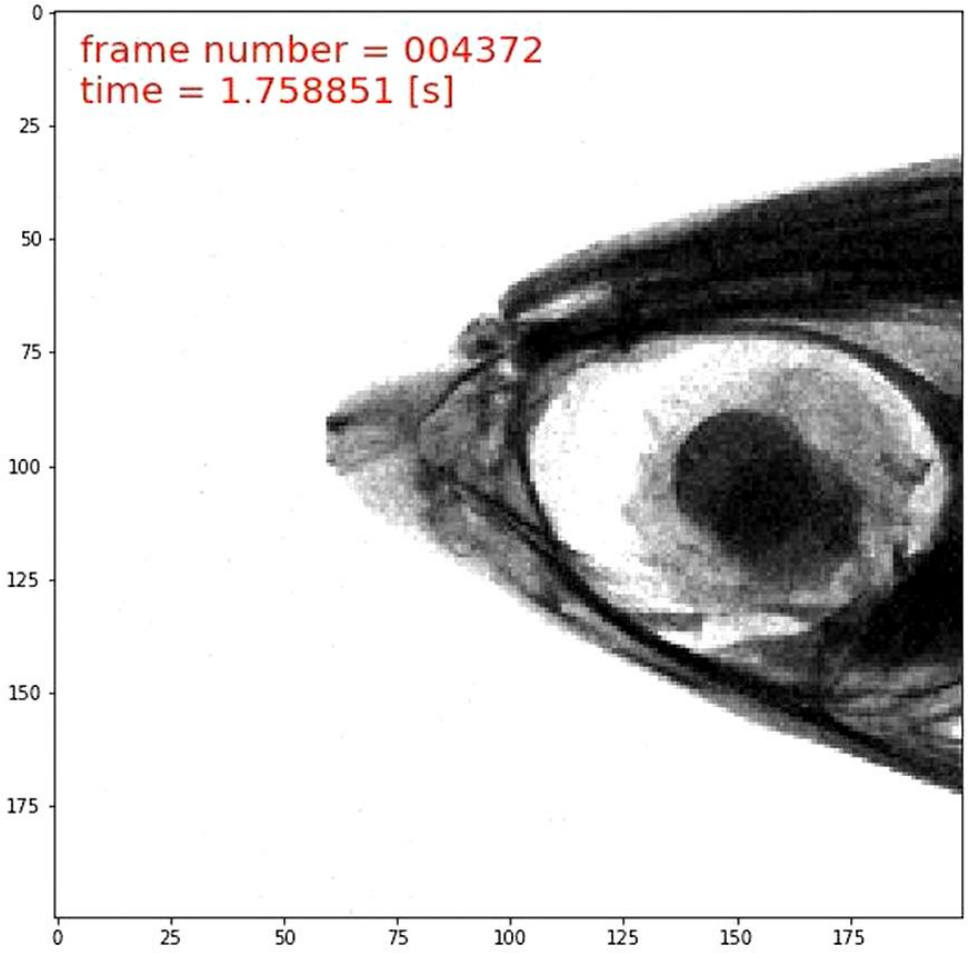
K. Ozaki, Y. Honjo,
T. Kudo, T. Hatsui

Micro Focus X-ray source (Cu target)
CITIUS Proto Camera、17.4 kfps、55 μs exposure/frame

Single Frame @ 17.4 kfps

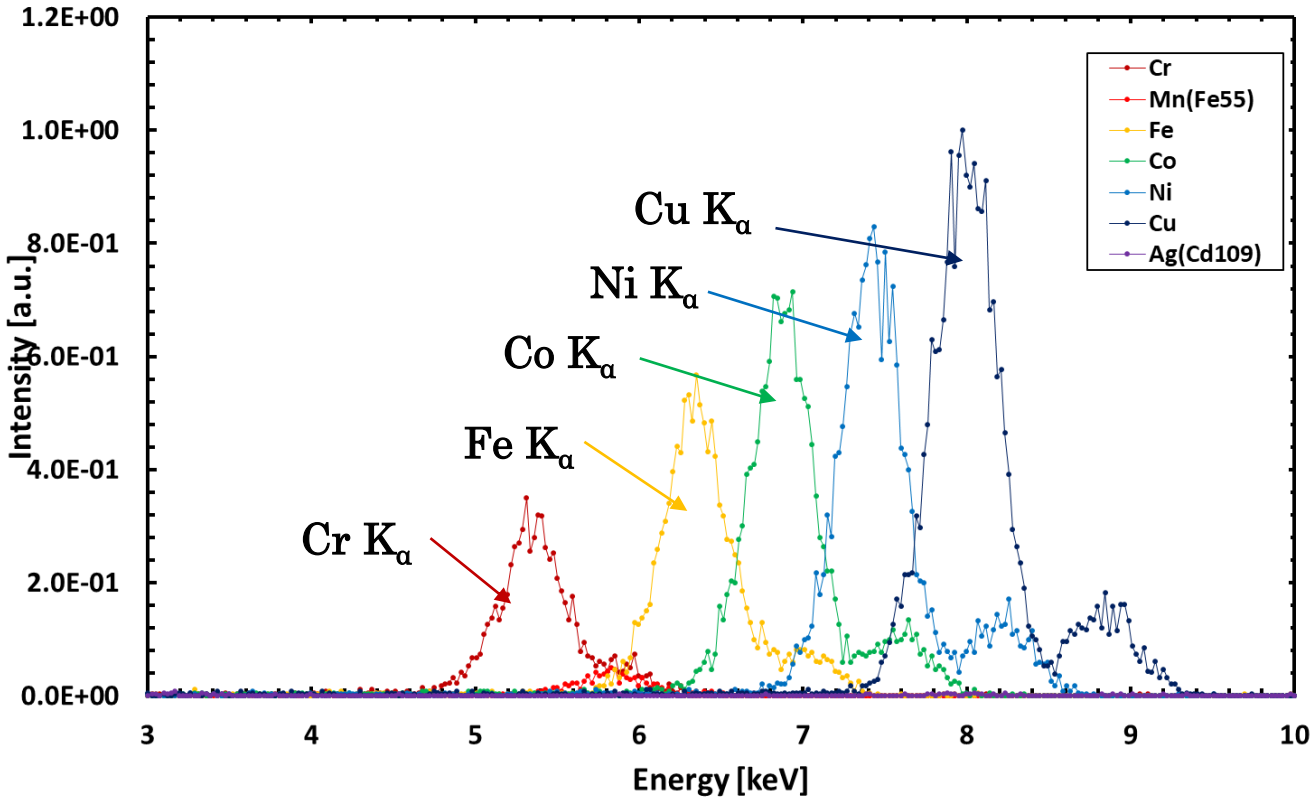


Accumulated Image



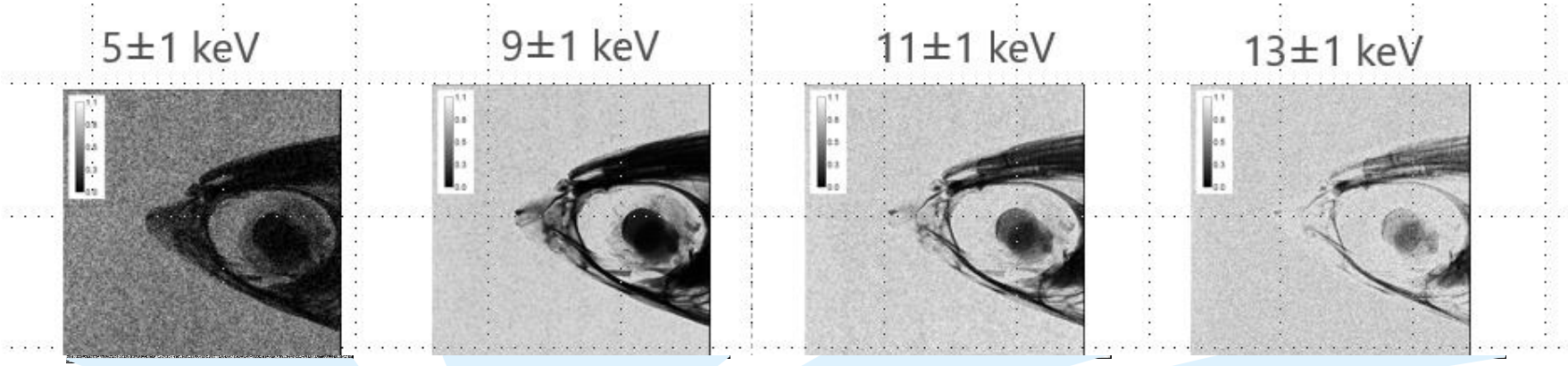
Energy Resolution demonstration

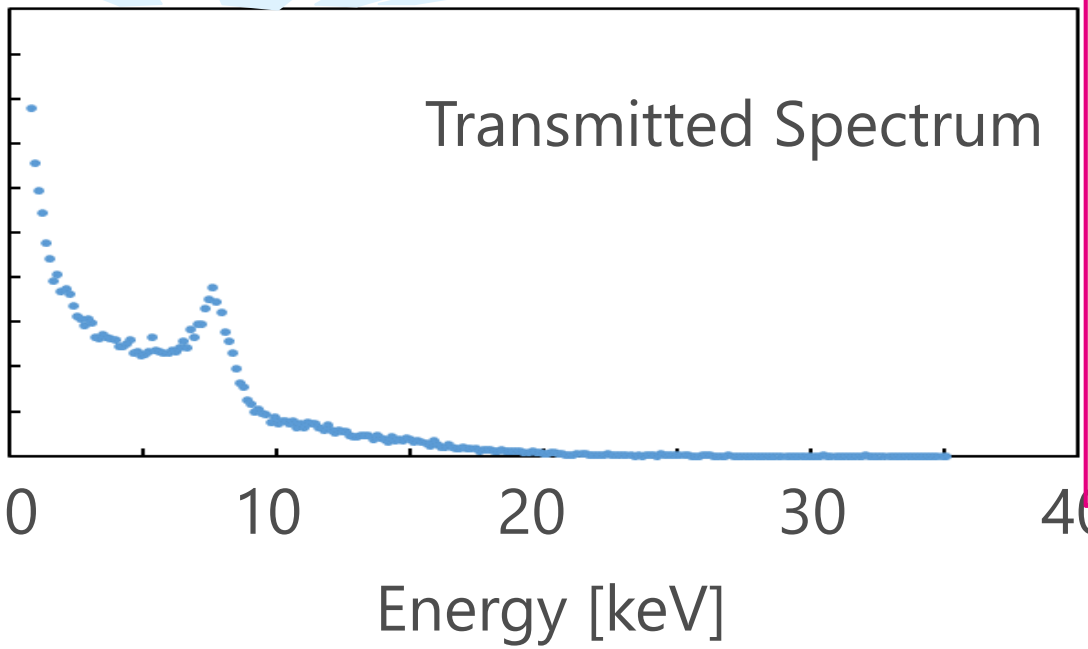
Data processing optimized for Energy Resolution



Element information can be extracted

Spectr- Imaging : Charge∝ Photon Energy





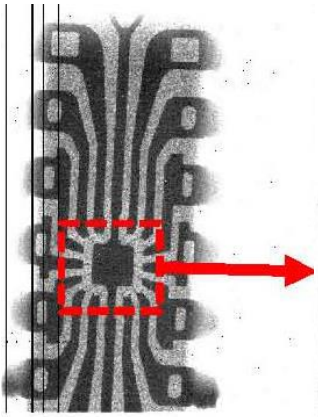
Analysis of 15,000 frames (～1 second)

Output of Analysis ～100 frames

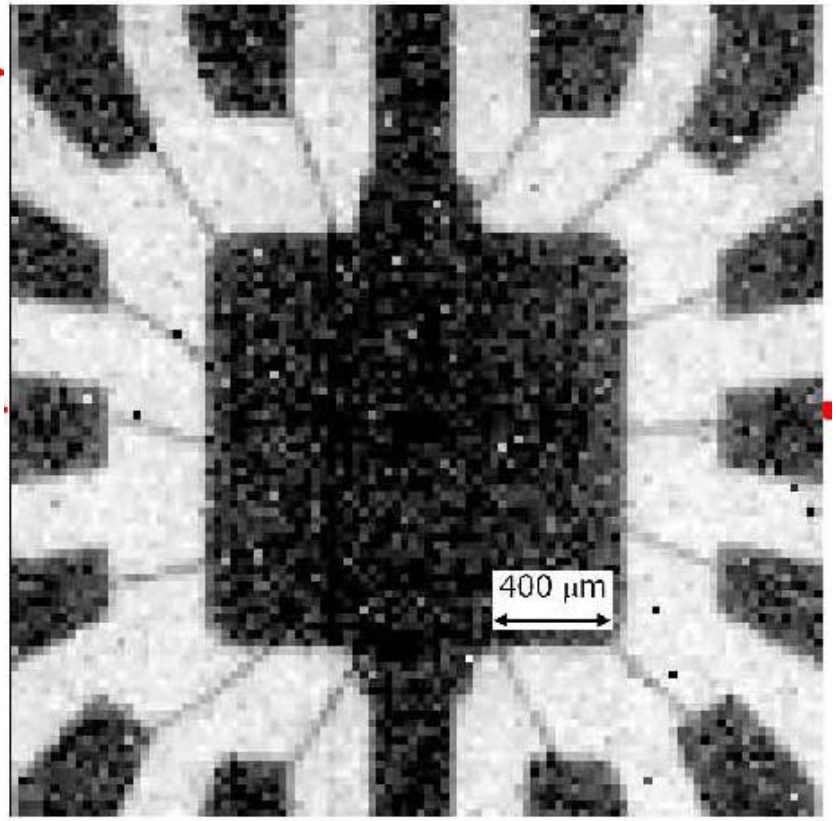
Sub-pixel Imaging: Charge Spread ➡ Sub pixel resolution

Demonstration by SOPHIAS-L

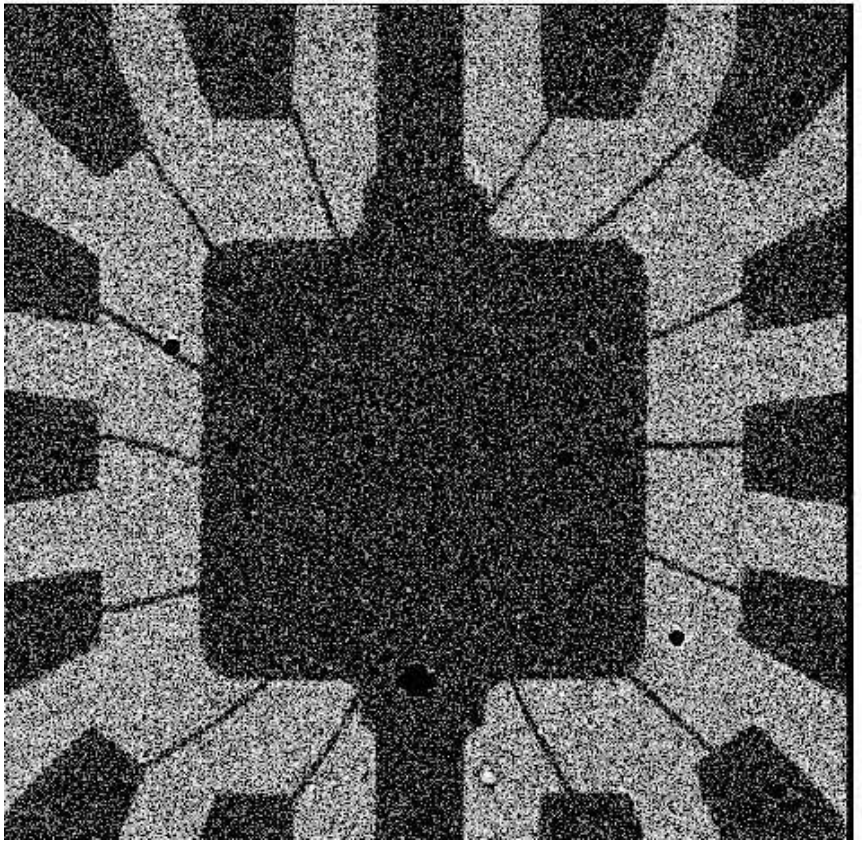
T. Kudo, T. Matsumoto et.al.,



30 μm□ Physical Pixel



6 μm□ Virtual Pixel



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Detector Output:
Conventional Photon Counting vs. Next Gen.Charge Integrating

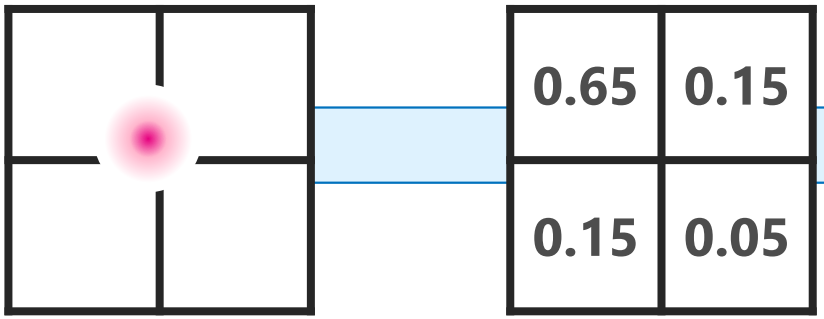
Conventional Photon Counting detector

Processed in silicon

Process partly in digital

Smaller data
at the expense
of loss of
information

Next Gen. Charge Integrating

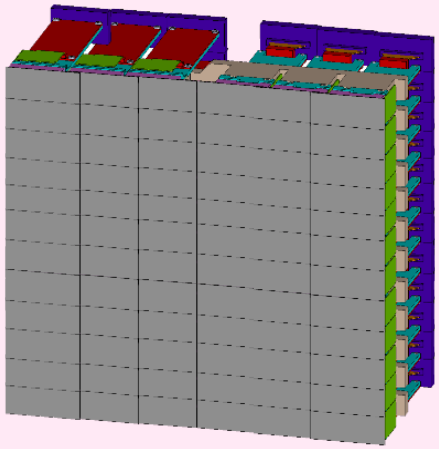


Process all in digital

Larger data
More information
(photon energy, sub-pixel etc.)

Data Output Rate from the Largest Detector System

Citius 20 Mpixels@17.4 kfps



Calibrated data stream
32 bits/pixel, 20 Mpixels, 17,400 frames/s

→ 0.348 Tpixels/s, 11.1 Tbps, **1.4 TB/s**

SPring-8 Operation senario
4000 hours/year
30 % data acquisition duty ratio

→ **6.0 EB/year**

SACLA Computer room

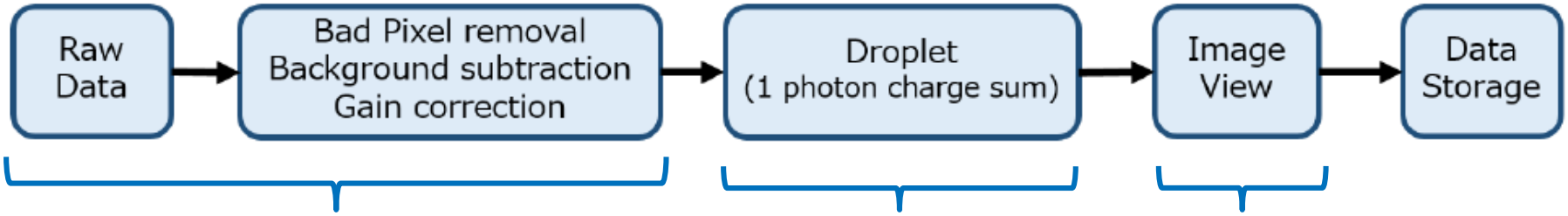
"Raw Data" Storage not practical

Store Processed Data by edge computing (eg.) "Accumulated" data

Implementation Example : SOPHIAS 1.9 Mpixel 30 fps

T. Matsumoto, T. Kudo, K. Ozaki

All implemented on CPU, 8 core parallel
Realtime calc. at 30 fps



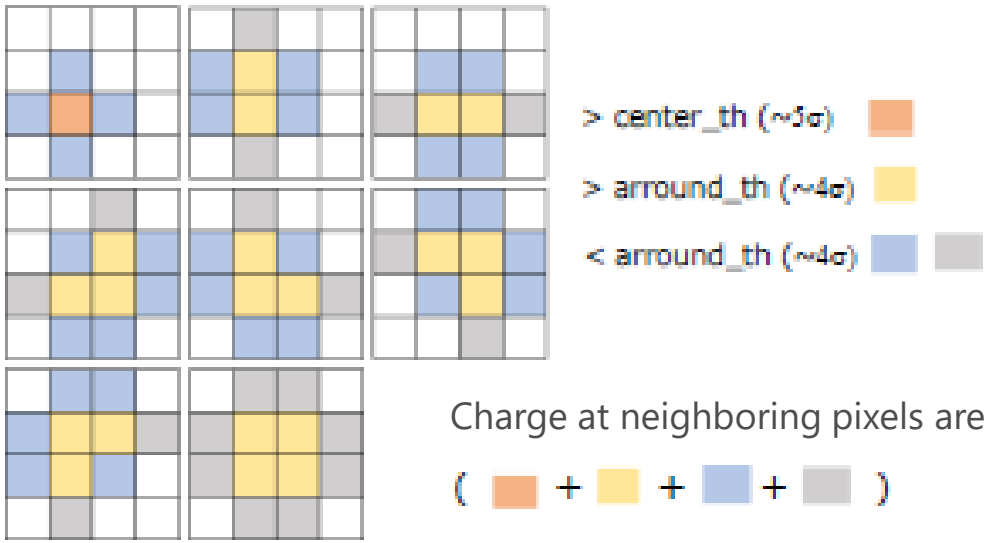
(almost)Pixel-wise Calc.

4x4 pixels Calc.

Data Reallocation
(Event building)

Input Data: 2 bits flag + 14 bits/pixel
Output Data: 32 bit floating

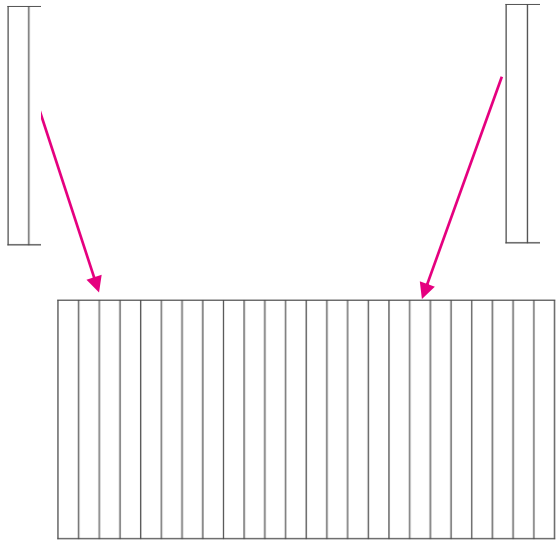
Pattern matching for 4x4 matrix



Charge at neighboring pixels are summed up

(+ + +)

Data from 24 ADCs



Single Frame data

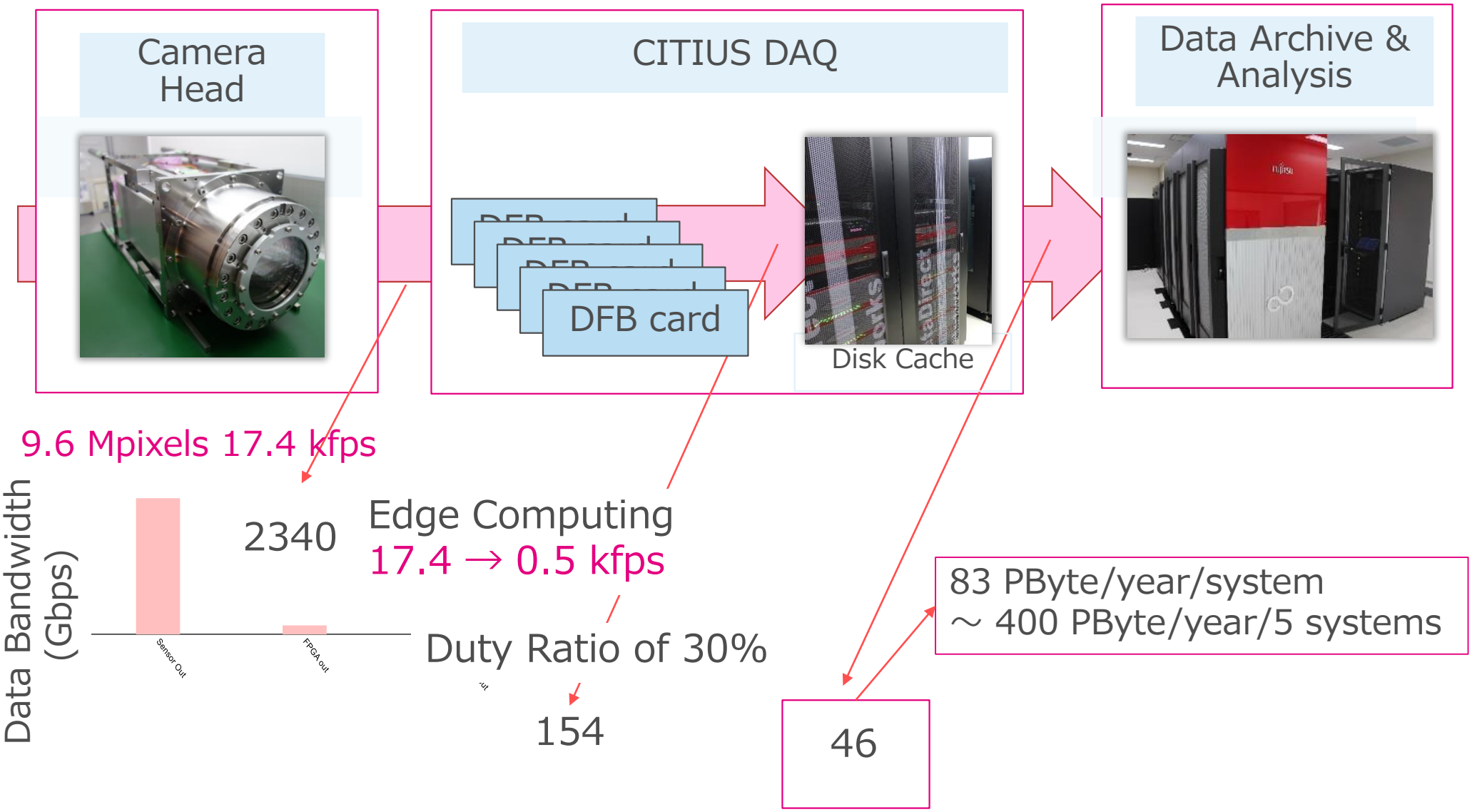
Performance Estimation

Detector	Pixel (Mpixels)	CPU threads	Calc. Frame Rate (fps)	Detector Frame Rate (fps)	Comment
SOPHIAS	1.9	8	100	30	Measurement (*)
Citius	0.28	8	679	17,400	calc.
	0.28	300	25,446	17,400	calc.
	20.16	**21,600**	25,446	17,400	calc.

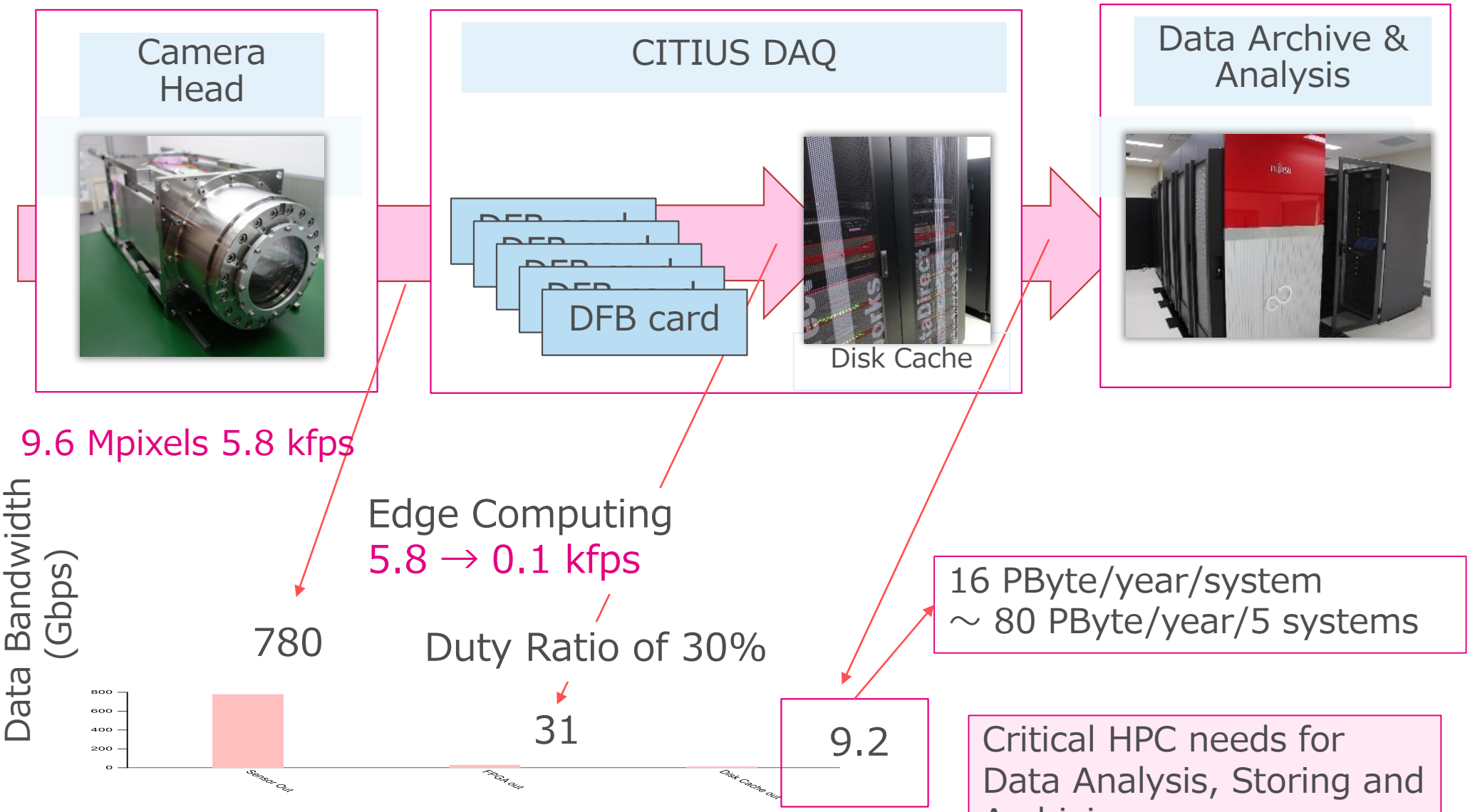
*) Processor : Intel Xeon E5-1640 v4, 3.6GHz(6 core, 12 thread), 15 MB cache

Edge calculations: significant cost.
Reduces the data size significantly without losing the information.
On-the-fly calculation will be a *MUST* in photon science.

Data Processing and Transfer
An example meeting objective Performance Requirements



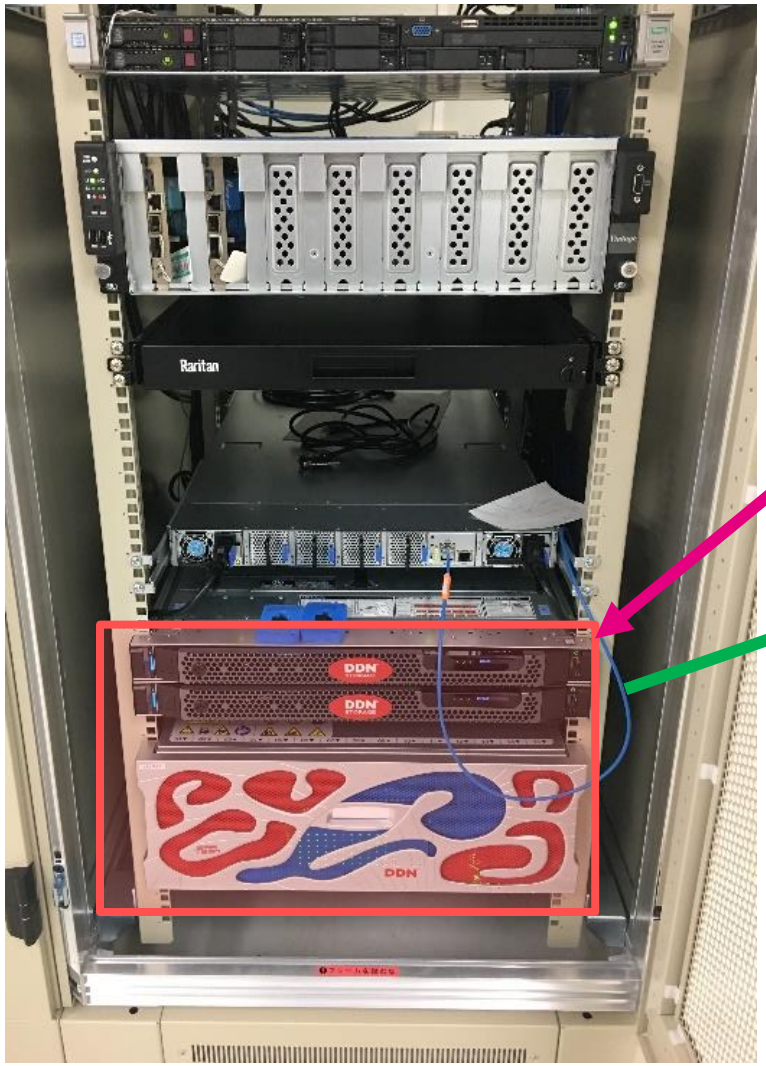
Data Processing and Transfer
An example meeting min. Performance Requirements



Data Visualization and Storage

M. Yamaga
Y. Joti

Edge Computing near detectors



Cache Storage
4 days ～ 300 TB

On-site Computing Resource

Off-site Computing Res.

Cloud

Data Generation Estimates at other facilities

- ESRF-EBS of Europe (ESRF)
  - Conservative estimate
  - 2021: 20 PB/year
  - 2022: 30 PB/year
  - 2023: 45 PB/year

- APS-U of U.S. (Argonne National Laboratory)
  - Now around 5-10 PB/year
  - Over 100 PB/year after upgrade in 2024
  - 50 Pflops at peak on-demand computing reserved for APS
  - Priority Area
    - Data management and workflow tools
    - Real-time data analysis capabilities
    - On-demand utilization of computing environments
    - Data storage and archival

Summary

2020: ESRF EBS in Europe
2024: APS-U in U.S.
202X: Petra IV in Germany
202X: SPring-8-II in Japan

- Photon science
  - X-ray delivered to samples will be x100-x1000 brighter in coming years
- CITIUS
  - **Next generation Detector** with Integration-type pixel & High-frame rate detector
    - **Frame rate 17.4 kfps (standard)**
  - Schedule: commissioning starts from **fall 2020**.
  - Jump from conventional counting detectors.
    - Detector Technology, and **data infrastructure**
  - Data rate may reach 6.0 EB/year/system
  - **With min. operation scenario, 80 PB/year/5 systems is estimated.**
    - Proper edge computing + HPC is mandatory
    - Compression, Information extraction…

Photon science will soon be an area of data science

Acknowledgement

- Members of RIKEN and JASRI
  - K. Nakajima, T. Tosue, K. Ozaki, Y. Honjo, K. Kobayashi, T. Kudo, **Y. Joti**, T. Sugimoto, T. Kameshima, Y. Inagaki, K. Fujiwara, **M. Yamaga**, **T. Abe**, T. Nakagawa, Y. Oyaki, M. Kimoto, M. Nakamachi

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- Nihon Gijyutsu Center
- Meisei Electric Co. Ltd.
- Yuji Matsuda (former RIKEN RSC, now at MIST Co,.Ltd)
- Nobukazu Teranishi, Takeo Watanabe, Hiroo Kinoshita (U. of Hyogo)
- Sony Semiconductor Solutions Cooperation
- Tokyo Electron Device Limited
- M. Yabashi, T. Ishikawa（RIKEN）
- Y. Imai, O. Sekizawa, N. Yasuda, K. Sugimoto, T. Uruga（JASRI）
- **K. Sato, K. Sano, T. Ueno, M. Kondo, J. Guo, S. Matsuoka (RIKEN R-CCS)**
- MEXT: Government subsidies for large-scale facilities
- METI/NEDO
  - Fukugo-Keisoku Project（複合計測）
  - Feasibility Study Program
    - T. Amemiya（JASRI）、A. Fujiwara（Kwansei Gakuin University）

Thank you for your attention