Data-analysis scheme and infrastructure at the X-ray free electron laser facility, SACLA

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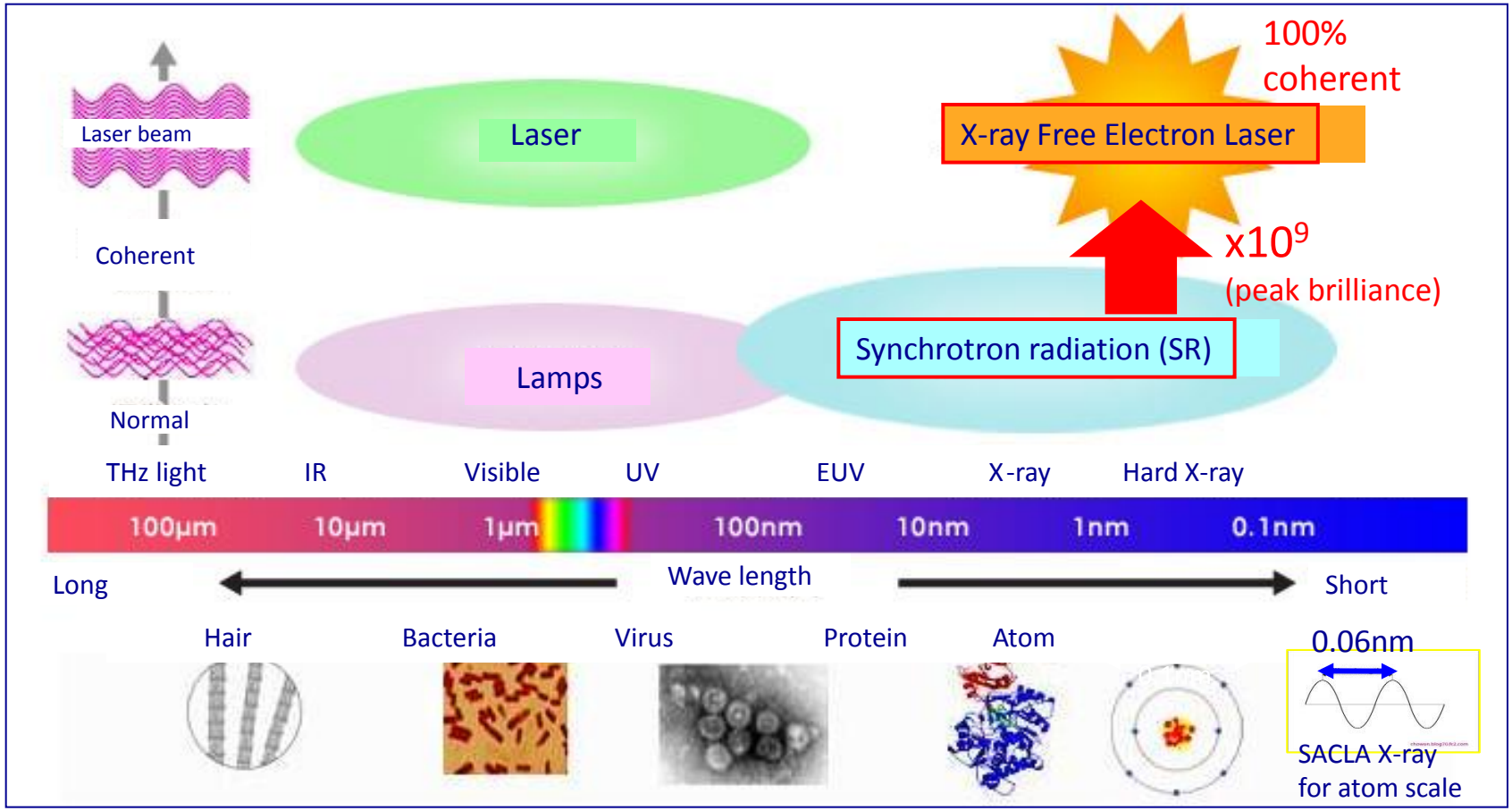
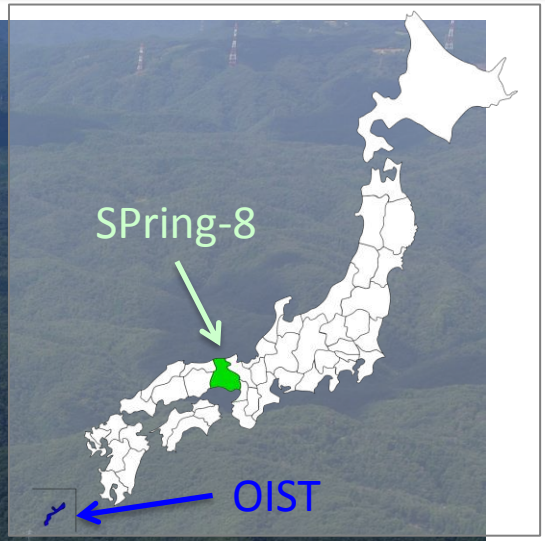
X-ray Free Electron Laser (XFEL)



SPring-8 and SACLA

SACLA is an X-ray Free Electron Laser (XFEL) facility, located in the SPring-8 campus, west region, Japan.



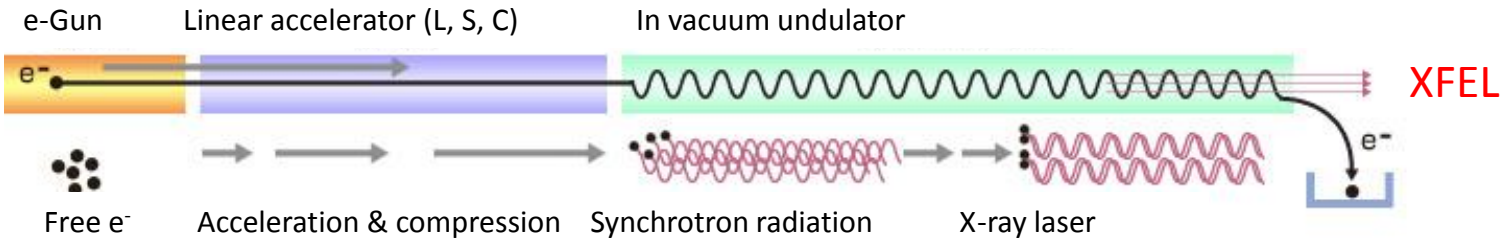
SPring-8, SR facility
(8-GeV storage ring)

SACLA, XFEL facility
(8-GeV linac)

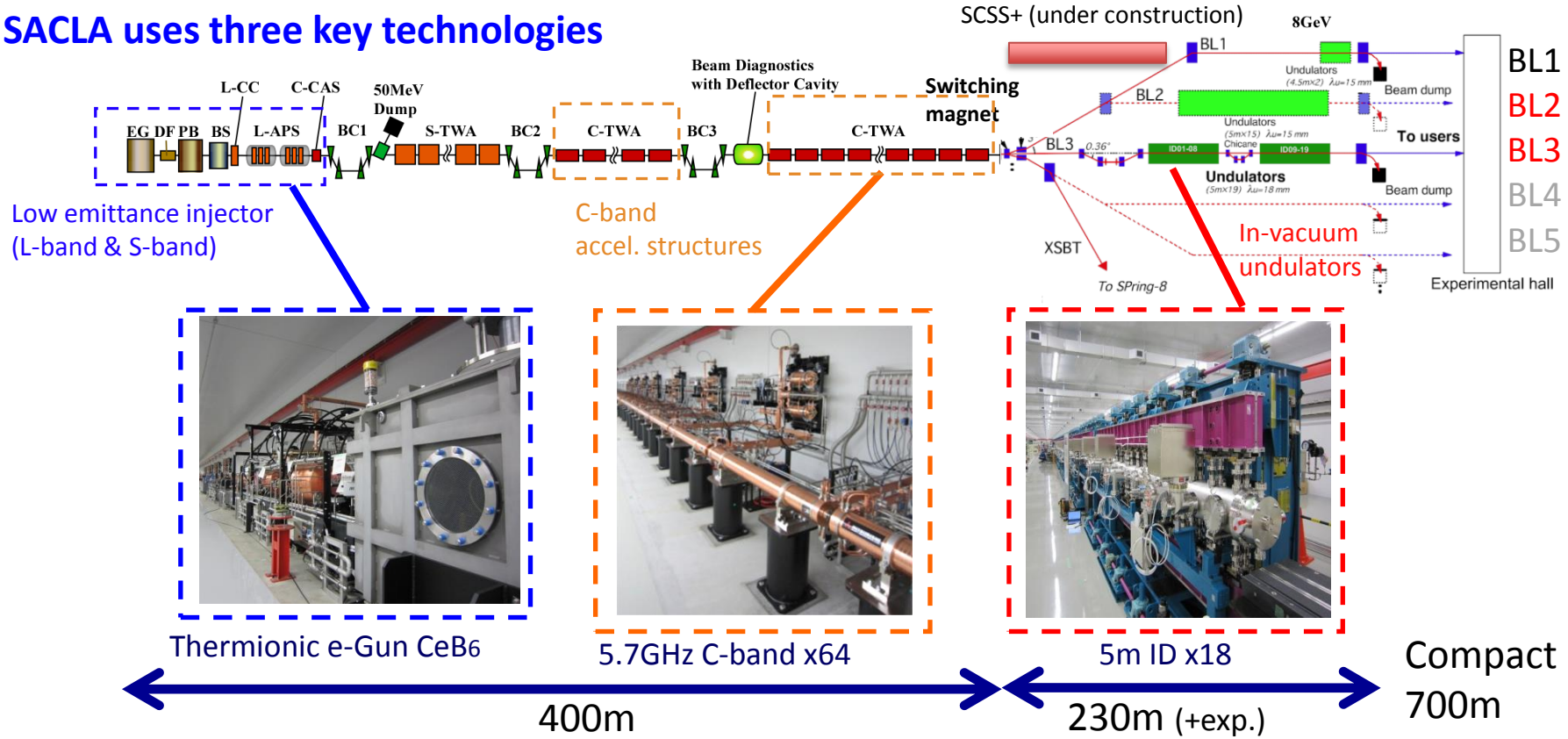
electron injector for SPring-8
(1-GeV linac and booster synchrotron)

XFEL lasing scheme at SACLA

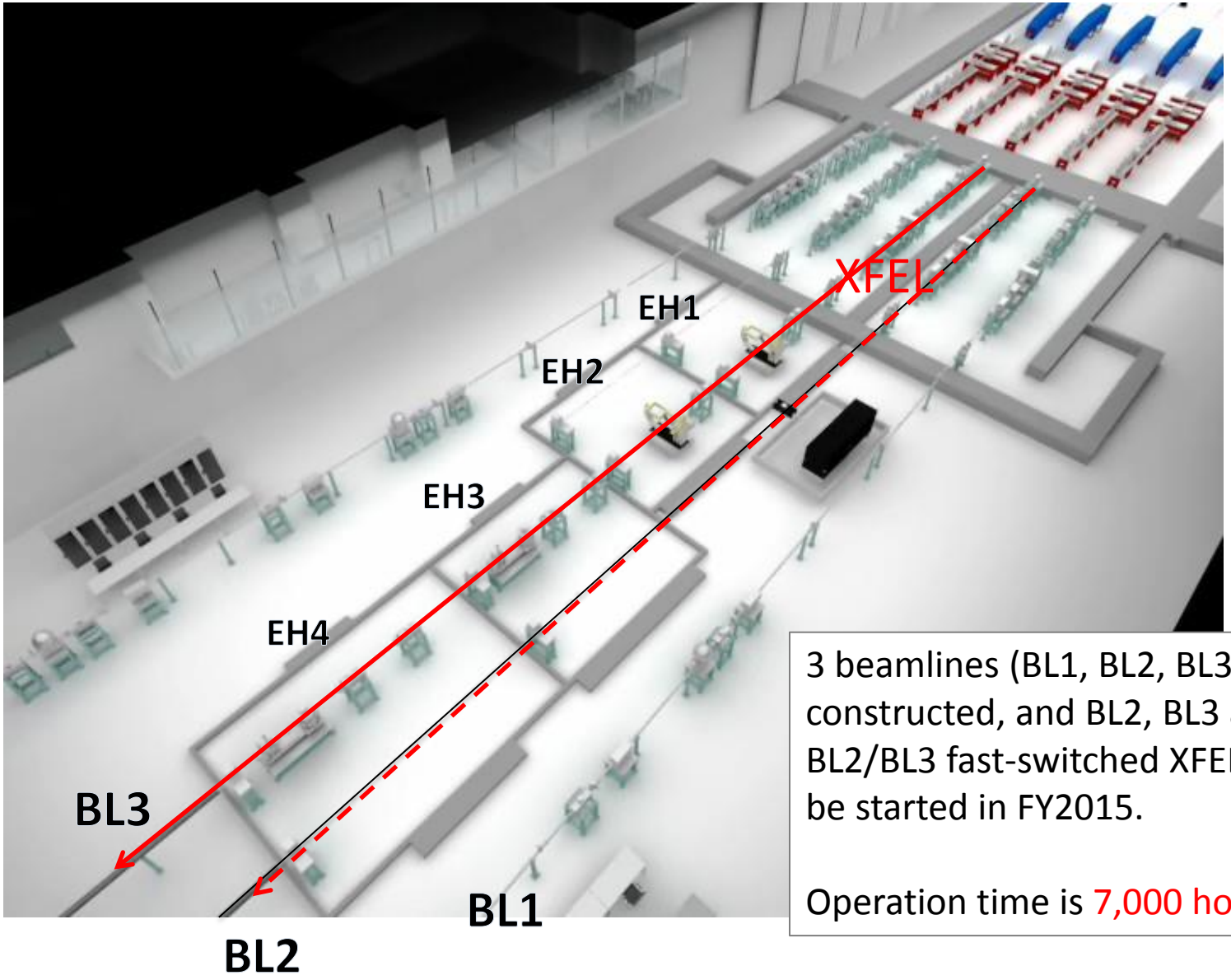
Lasing scheme



SACLA uses three key technologies



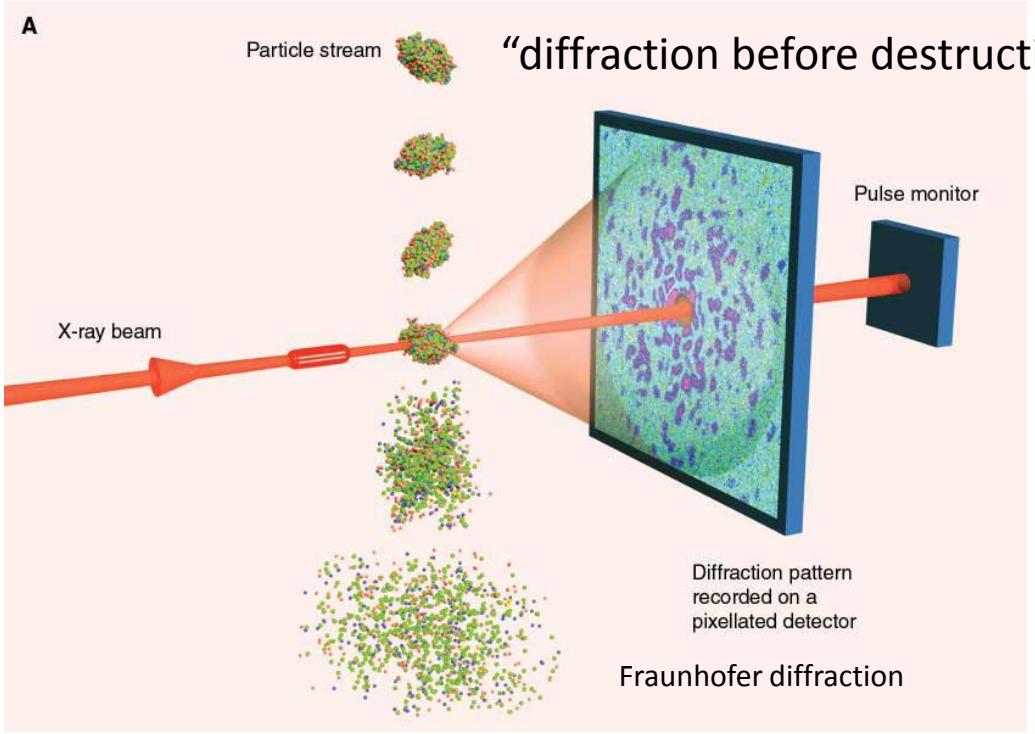
Beamlines

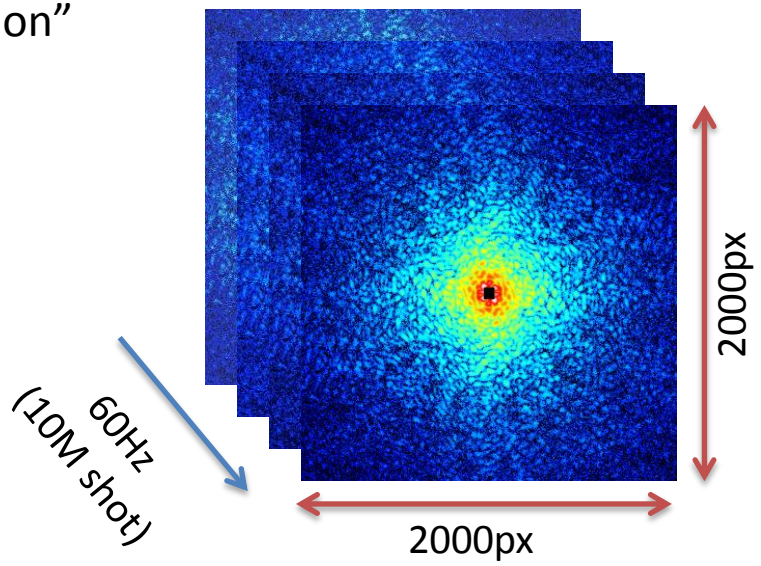


3 beamlines (BL1, BL2, BL3) have been constructed, and BL2, BL3 are in operation. BL2/BL3 fast-switched XFEL distribution will be started in FY2015.

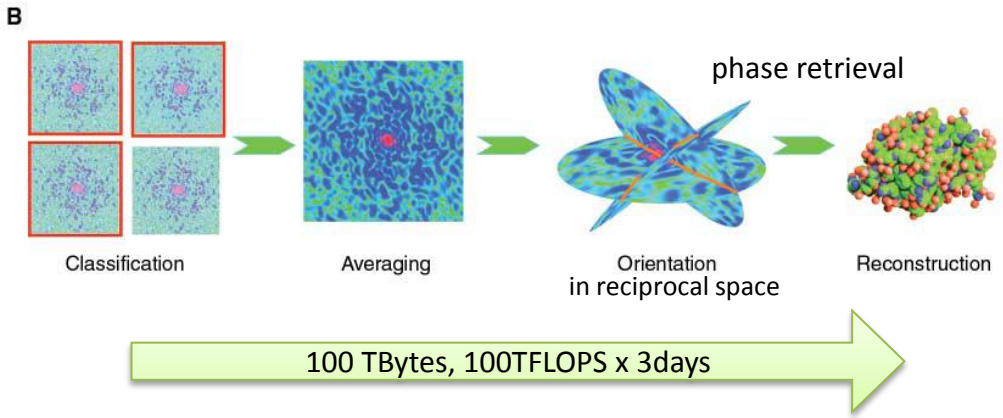
Operation time is 7,000 hour/year.

Coherent X-ray Diffraction Imaging (CXDI)





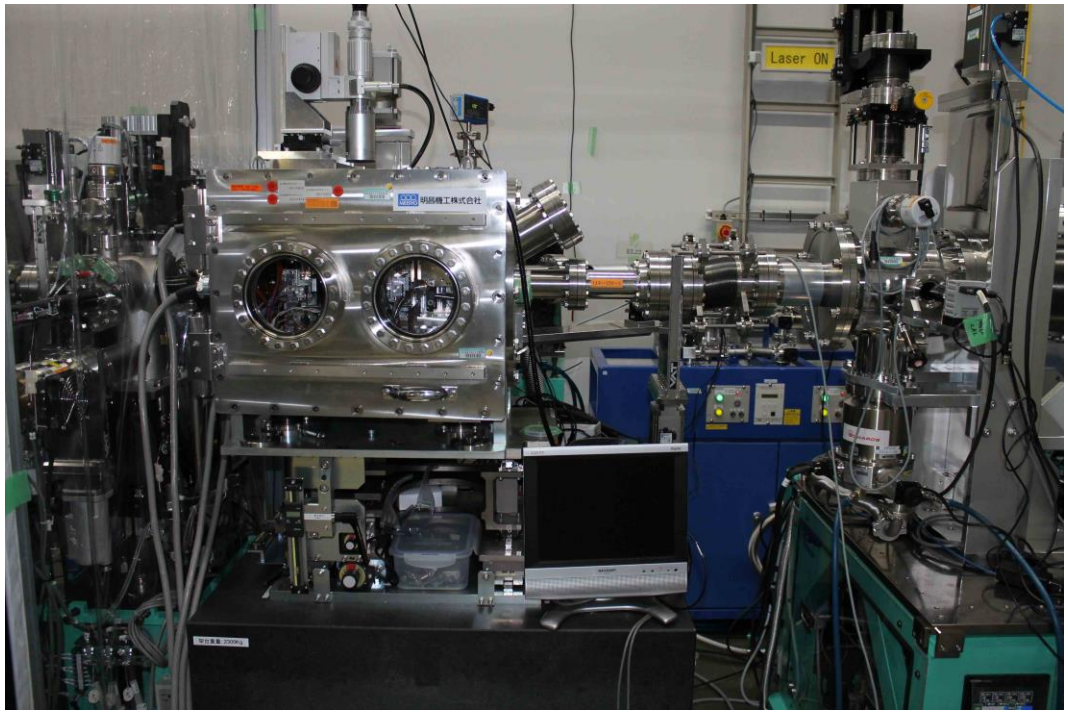
1 M shots of diffraction images are necessary to reconstruct 3-D structure.
Considering XFEL hit rate on sample, 10 M shots data are required.
-> more than 100 TB storage per sample



To reconstruct 3-D image in real space, we must analyze relationship between 1 M images.
XFEL experiments requires heavy computing resources.
-> 100 TFLOPS x 3 days (per sample)

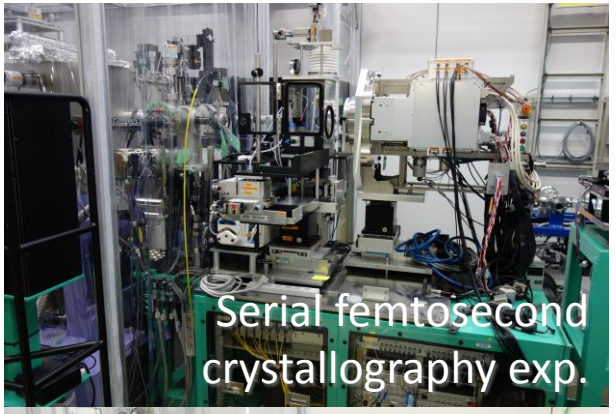
K. J. Gaffney and H. N. Chapman, Science 316, 1444 (2007)

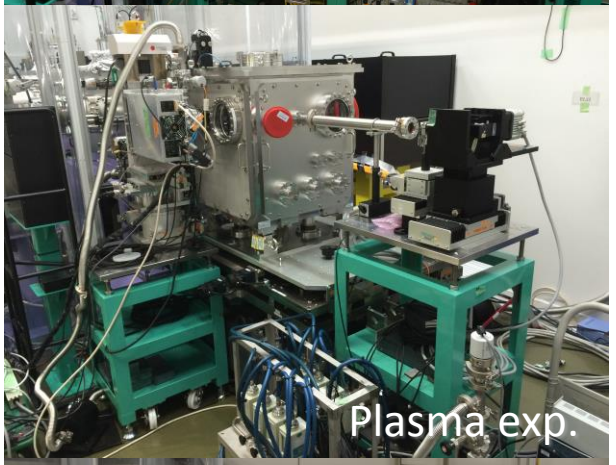
Experimental setups

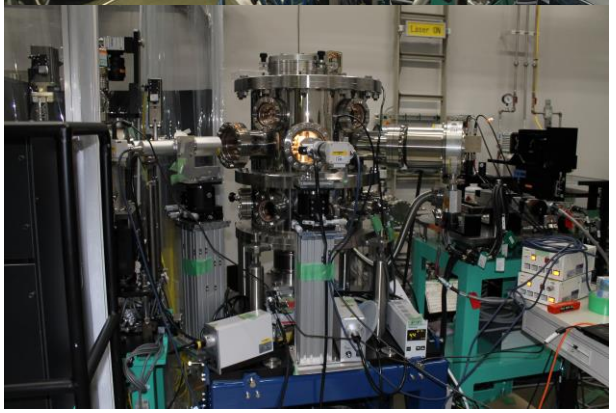


CXDI Experiment

Experiment changes every few days.
We must setup detectors and DAQs as fast as possible.





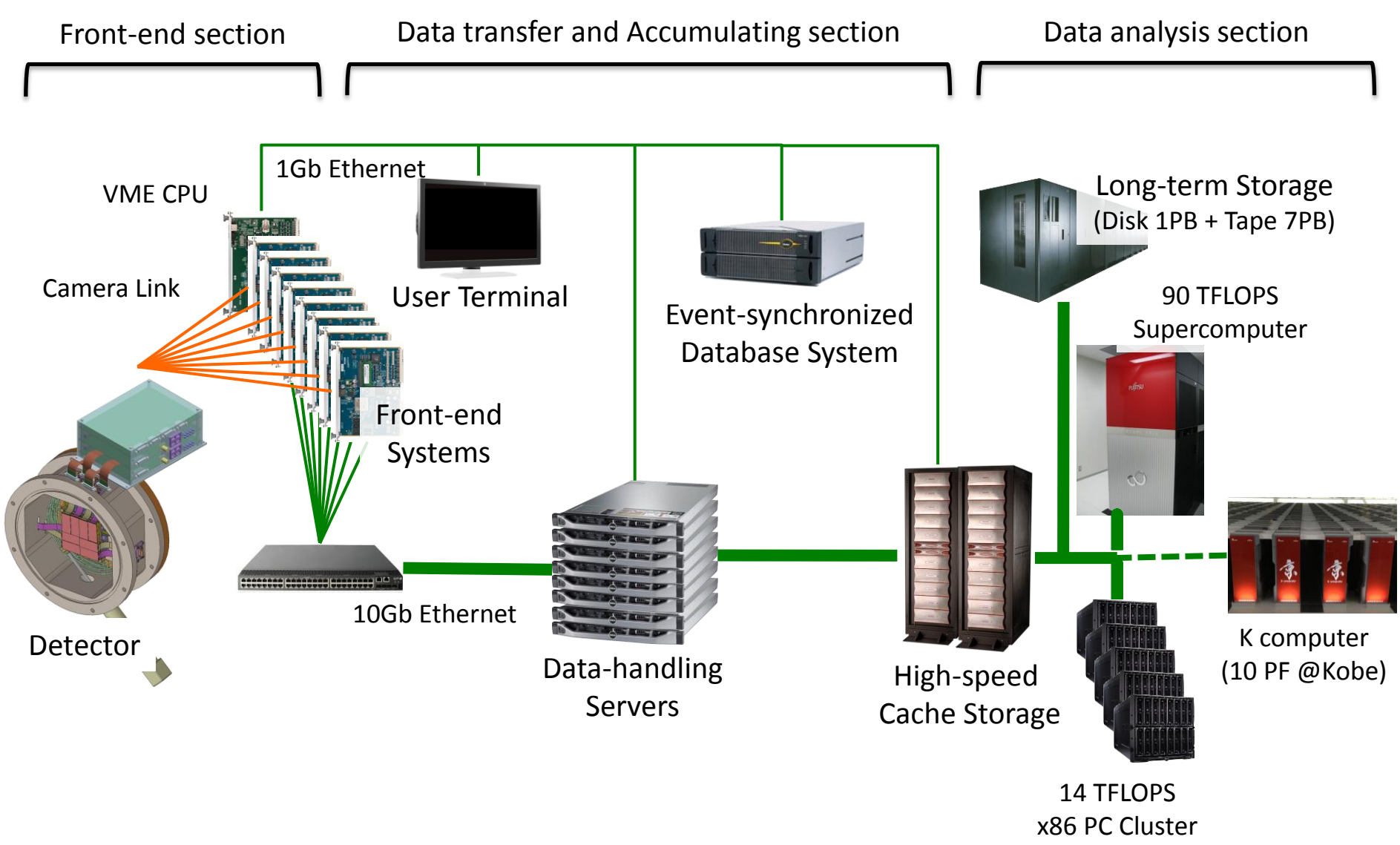


Requirement for the DAQ and the analysis systems

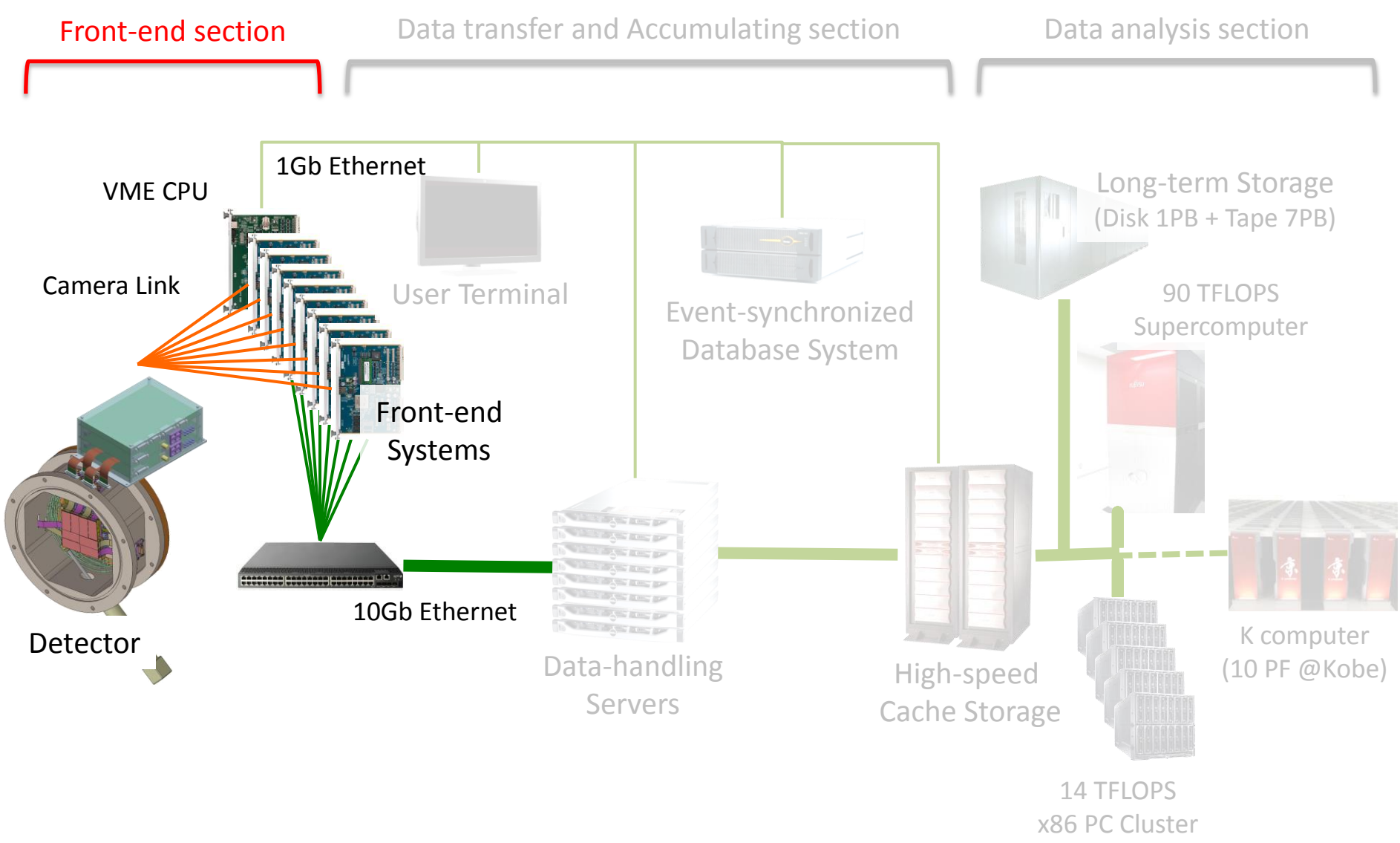
- Images are accumulated at 6 Gbps data rate
  - 12 MBytes (12 sensors) at 60 Hz repetition
- One experimental sample requires 120 TBytes storage
  - 12 MBytes x 10 M shots
- Short experimental period
  - Sample and/or detector setup change every few days
  - Users want to use the SACLA as a commercial microscope. (System tuning / DAQ is not their science)
- Analysis should be faster than the DAQ data rate
  - 10 TFLOPS for run-by-run analysis and pre processing (10M -> 1M)
  - 100 TFLOPS for 3-D structure reconstruction within a few days.

DAQ and Analysis System at SACLA

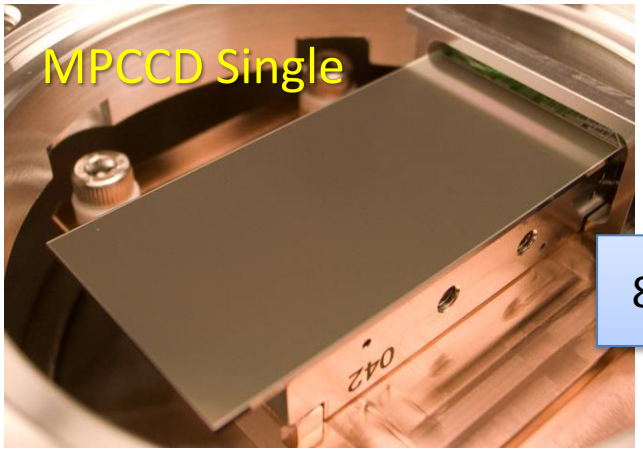
SACLA DAQ and Analysis System



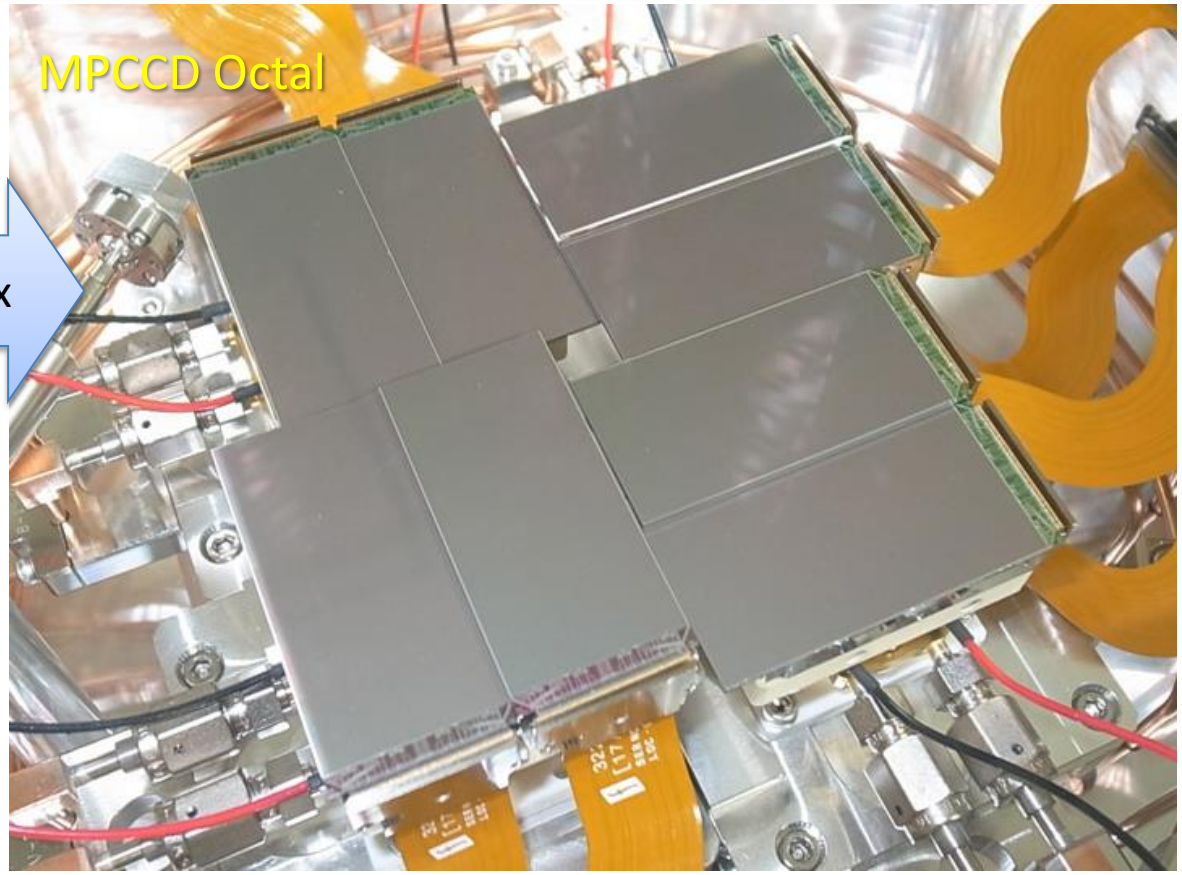
Detector Front-end System



MPCCD sensor



8x



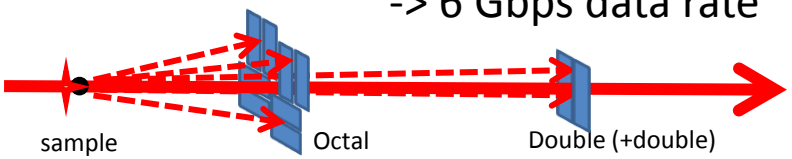
MPCCD sensor
(512 x 1024 px, 16bit depth)

Trigger =
accelerator repetition (60 Hz)
-> data rate is 0.5 Gbps/sensor

T. Kameshima, et al., Rev. Sci. Instrum. 85, 033110 (2014).

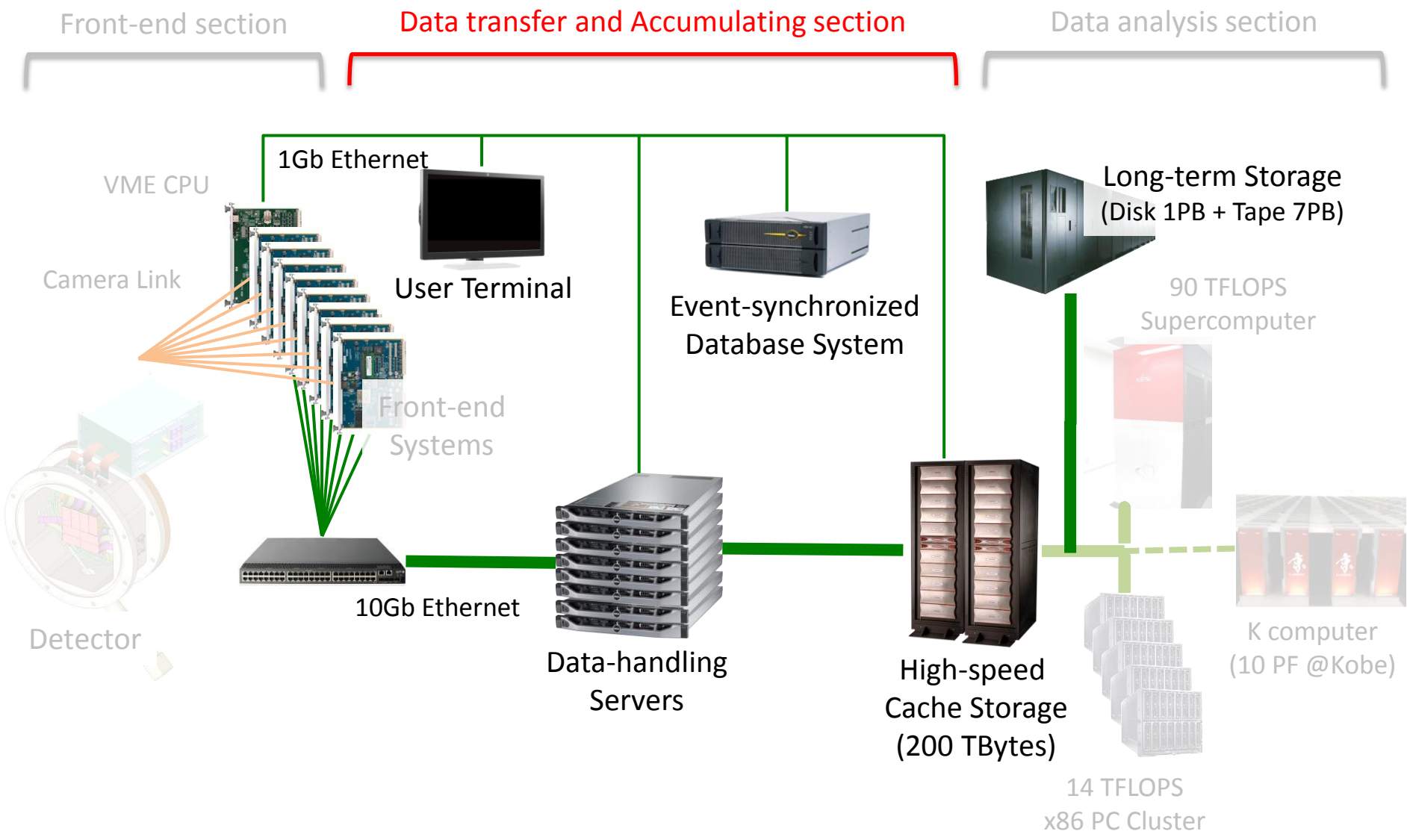
To avoid radiation damage from direct XFEL beam, 8+2+2 sensors are installed offset from the beam line.

-> 6 Gbps data rate

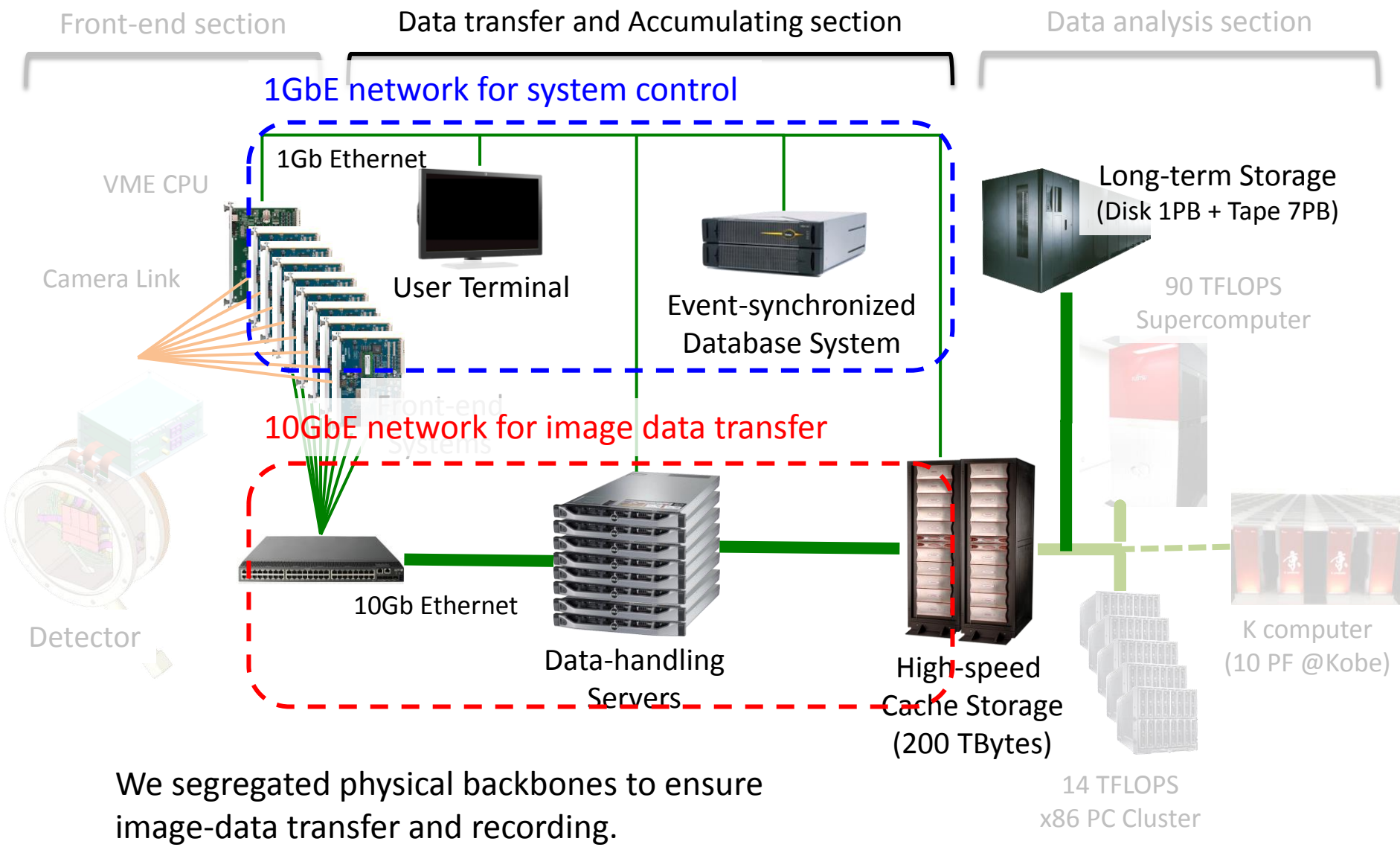


Note: All images (including junk) are recorded. Because it is difficult to determine reduction condition within few-day experimental period.

DAQ Network

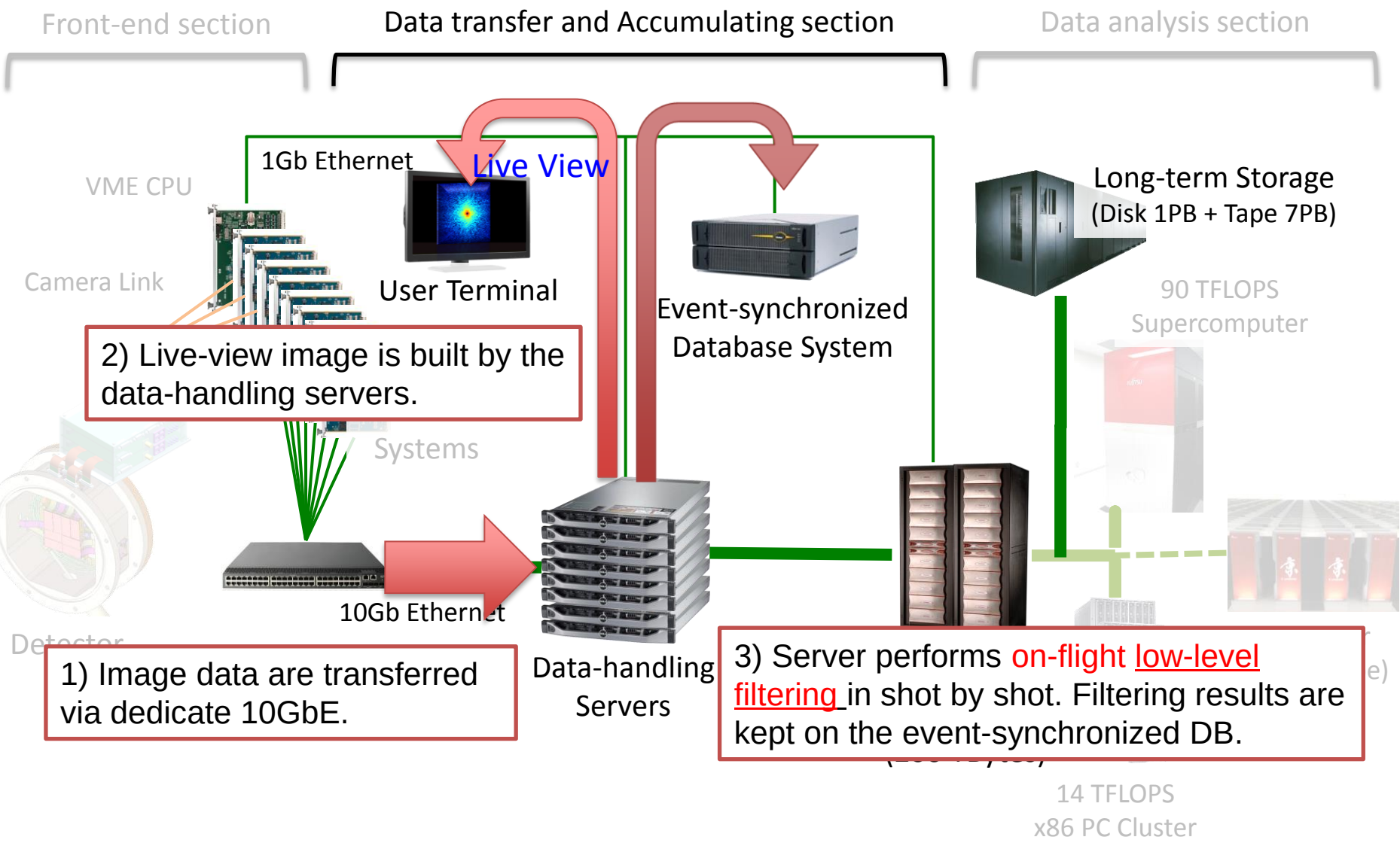

Front-end section
Data transfer and Accumulating section
Data analysis section
1Gb Ethernet
VME CPU
Camera Link
User Terminal
Event-synchronized
Database System
Long-term Storage
(Disk 1PB + Tape 7PB)
90 TFLOPS
Supercomputer
Front-end
Systems
Detector
10Gb Ethernet
Data-handling
Servers
High-speed
Cache Storage
(200 TBytes)
K computer
(10 PF @Kobe)
14 TFLOPS
x86 PC Cluster

DAQ Network

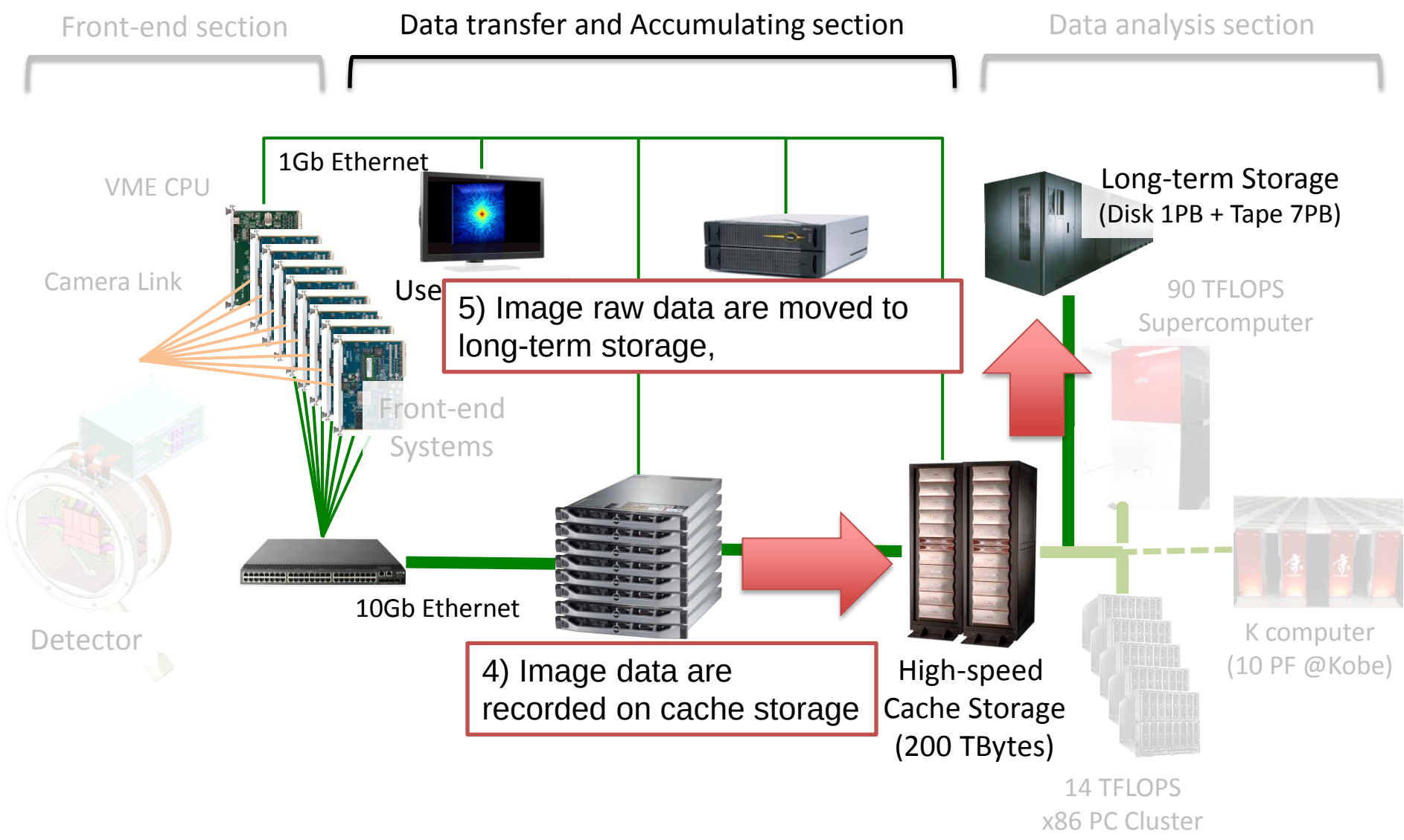


We segregated physical backbones to ensure image-data transfer and recording.

DAQ Data flow



DAQ Data flow



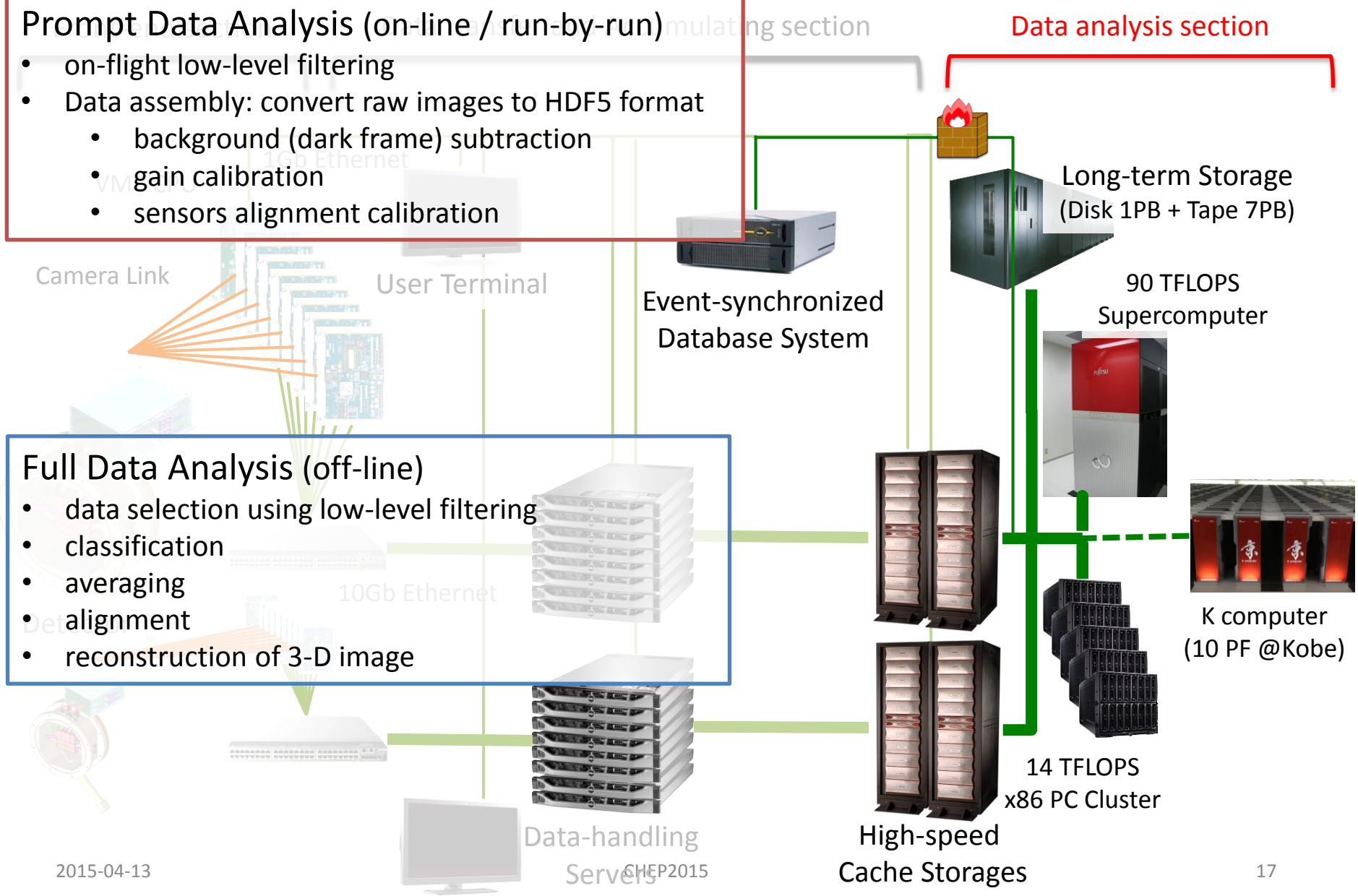
Data analysis section

Prompt Data Analysis (on-line / run-by-run)

- on-flight low-level filtering
- Data assembly: convert raw images to HDF5 format
  - background (dark frame) subtraction
  - gain calibration
  - sensors alignment calibration

Full Data Analysis (off-line)

- data selection using low-level filtering
- classification
- averaging
- alignment
- reconstruction of 3-D image



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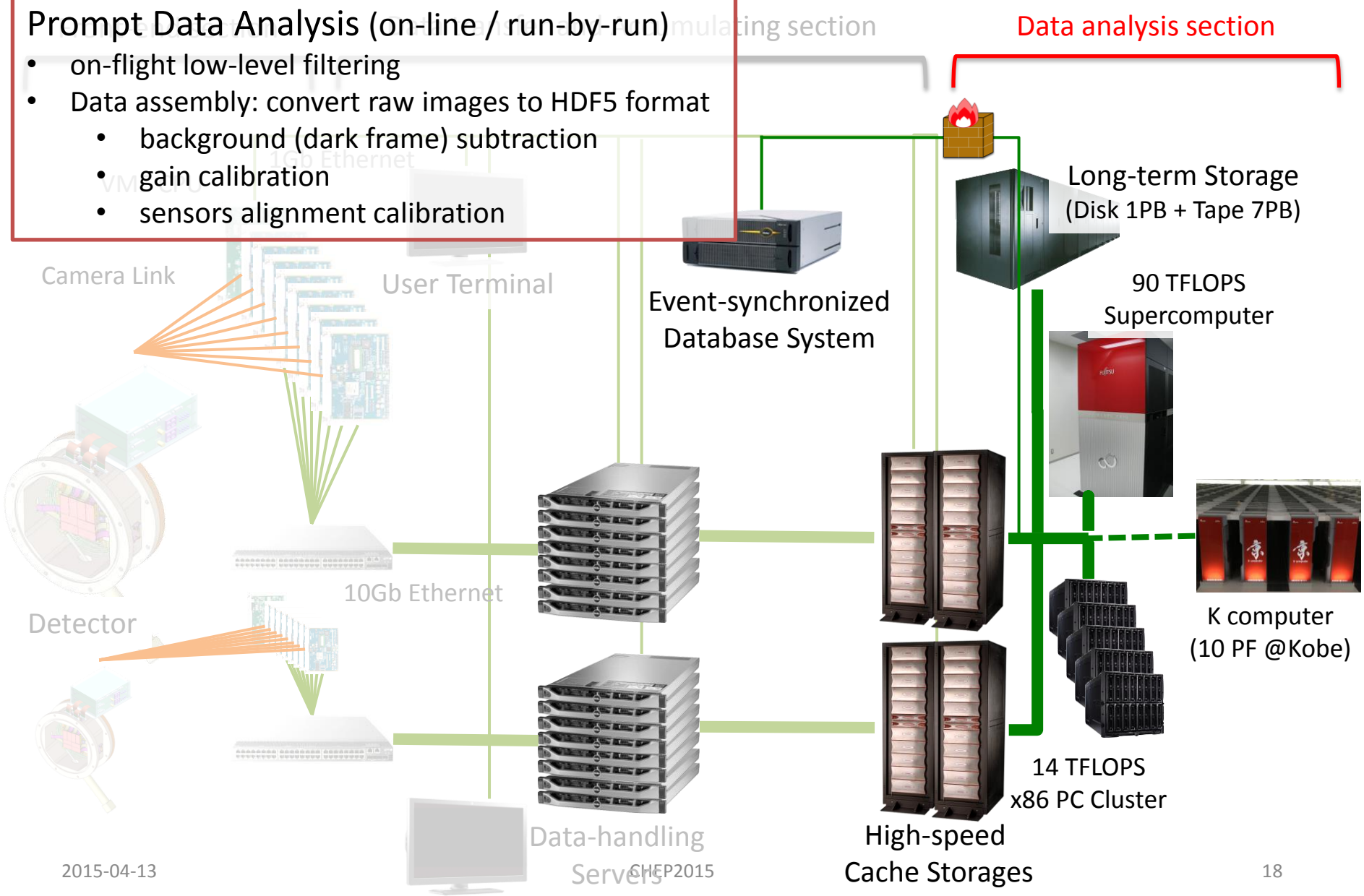

Prompt data analysis

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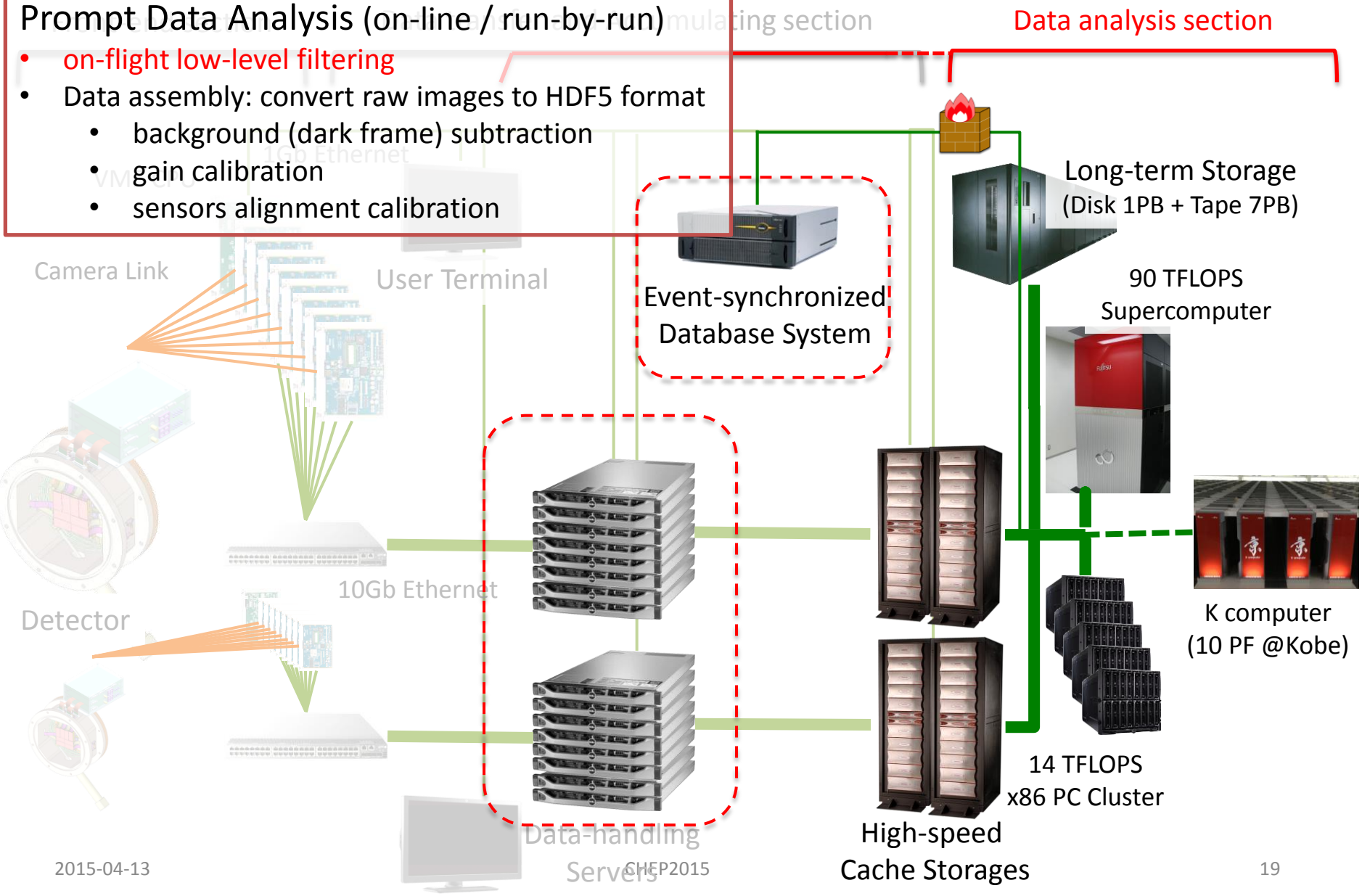
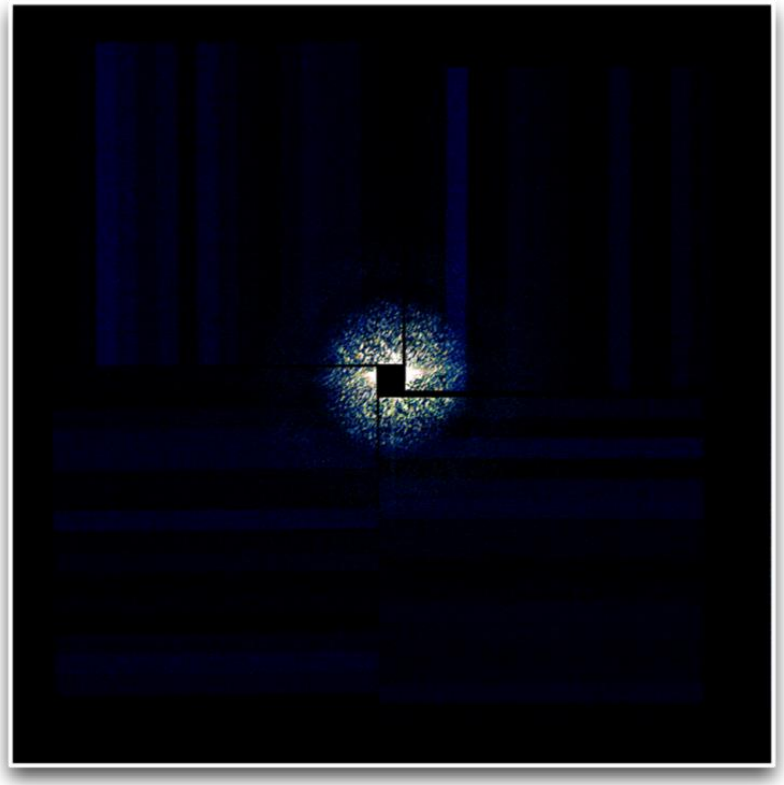


Prompt data analysis: Low-level filtering

To reduce latter computing load, we want to identify candidates of GOOD event.



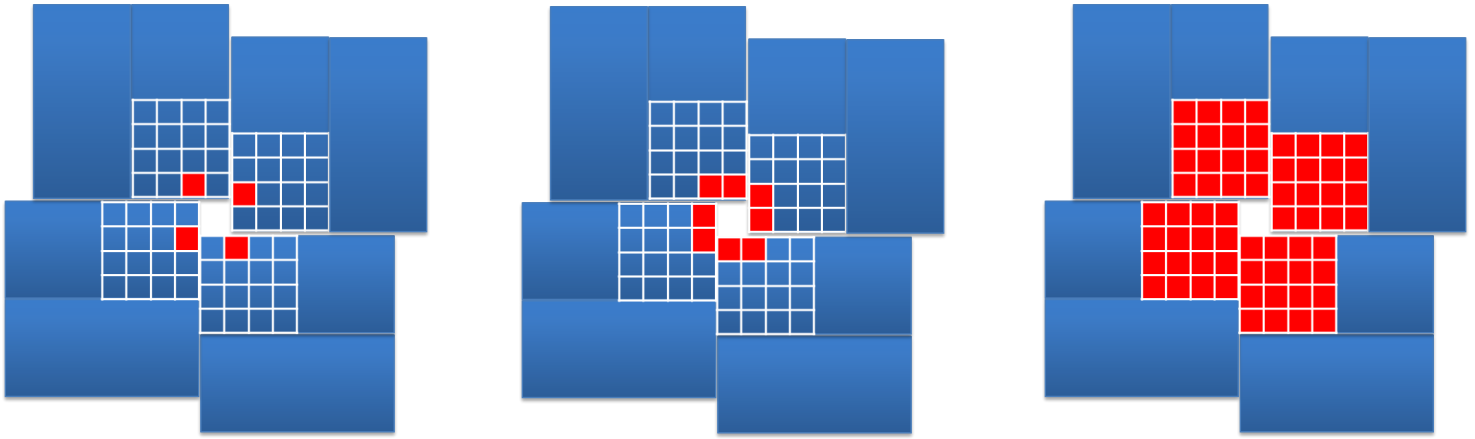
Exapmle of GOOD event
(diffraction pattern)

Example of BAD event
(scattered by water)

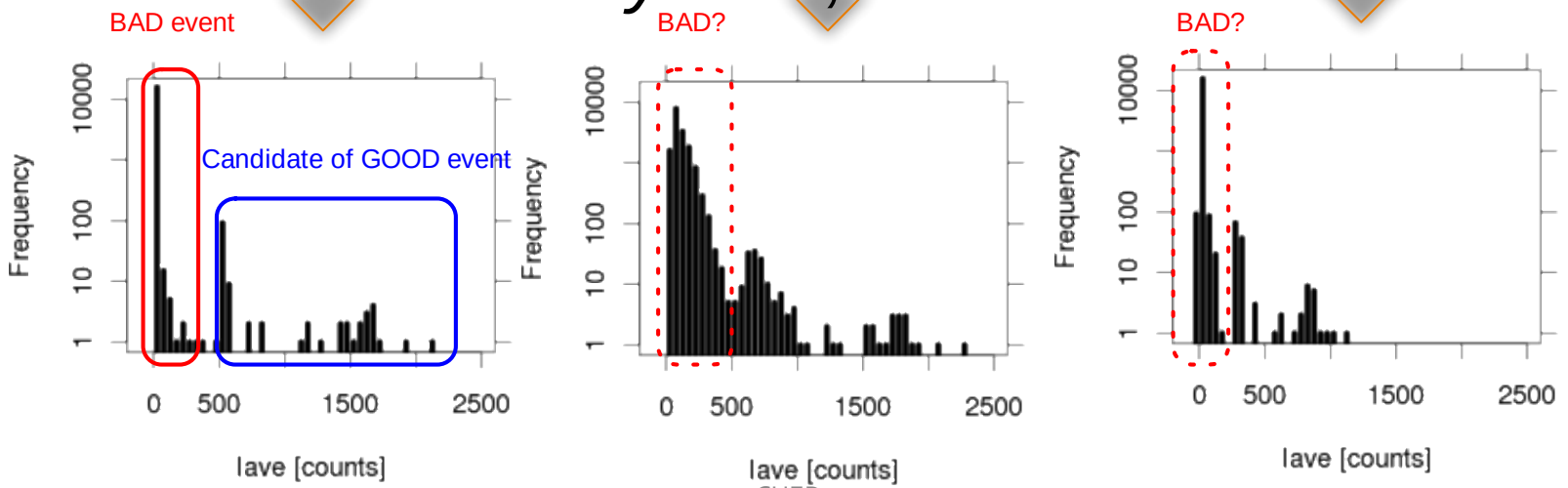
Prompt data analysis: Low-level filtering

To reduce latter computing load, we want to identify candidates of GOOD event.
Intensities in the mesh are recorded on event-synchronized DB.
By selecting ROI, we can distinguish GOOD event from bad event.

Region of Interest (ROI)



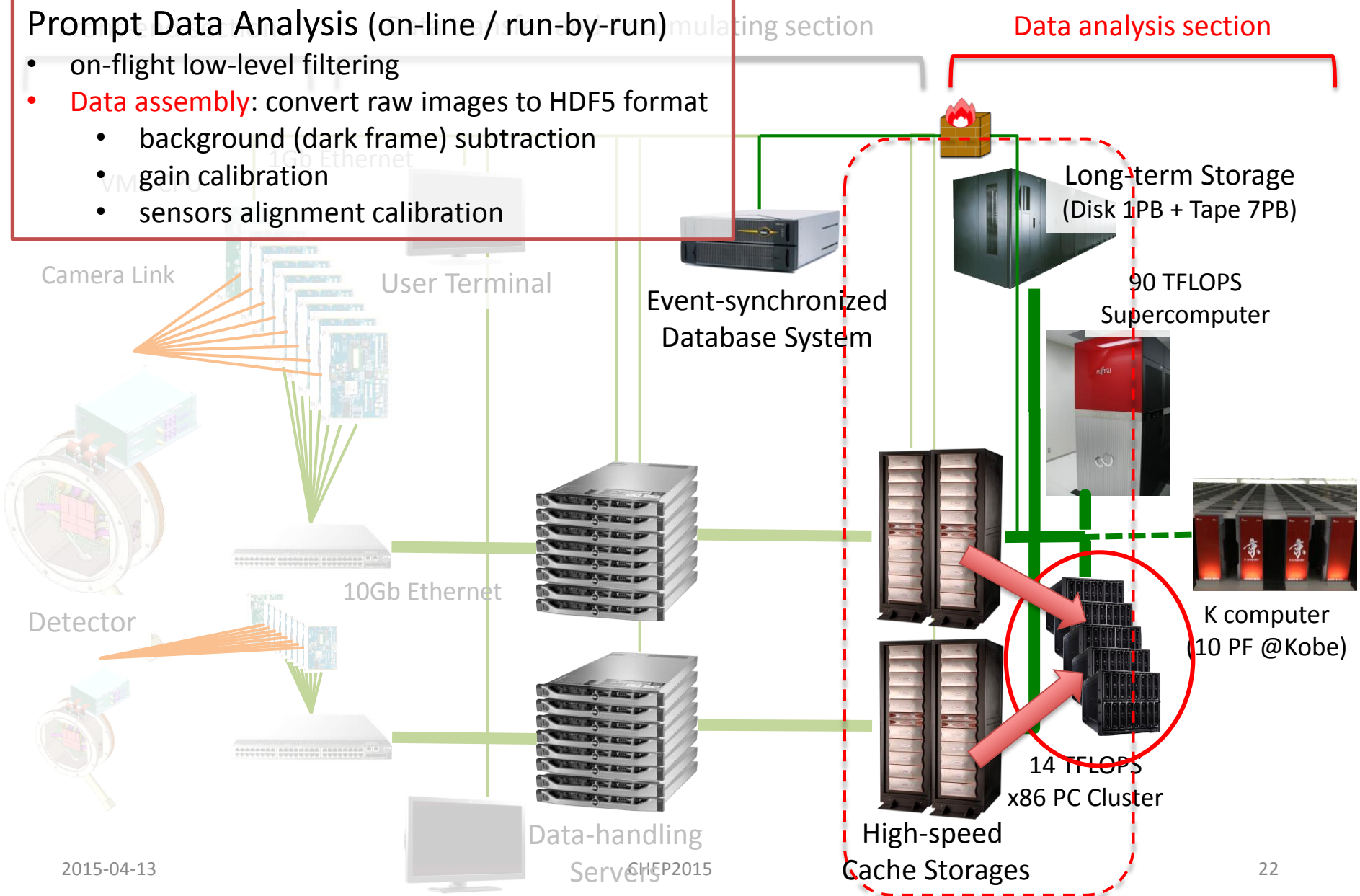
Analyze 13,000 event



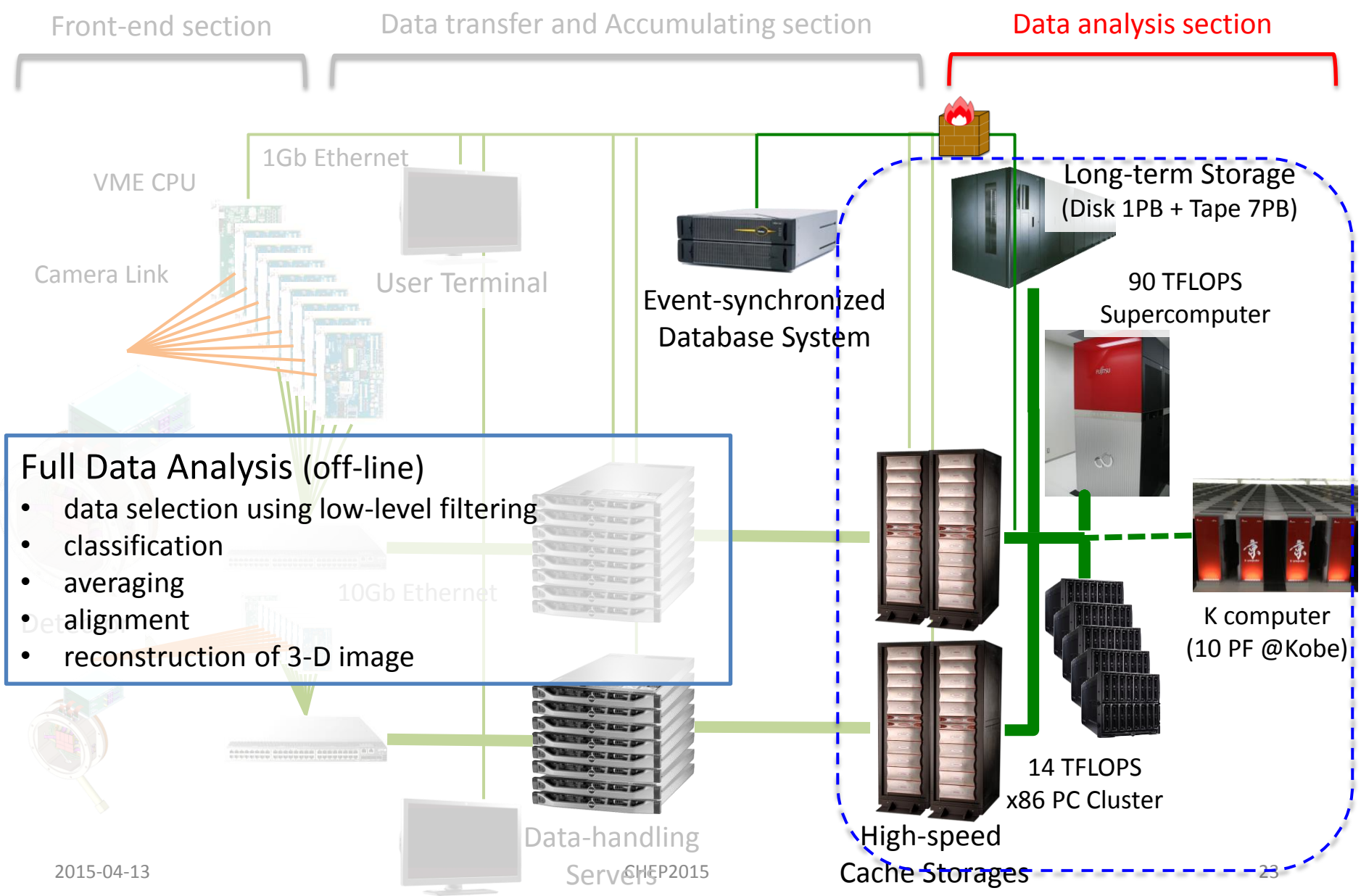
Prompt data analysis

Prompt Data Analysis (on-line / run-by-run)

- on-flight low-level filtering
- Data assembly: convert raw images to HDF5 format
  - background (dark frame) subtraction
  - gain calibration
  - sensors alignment calibration



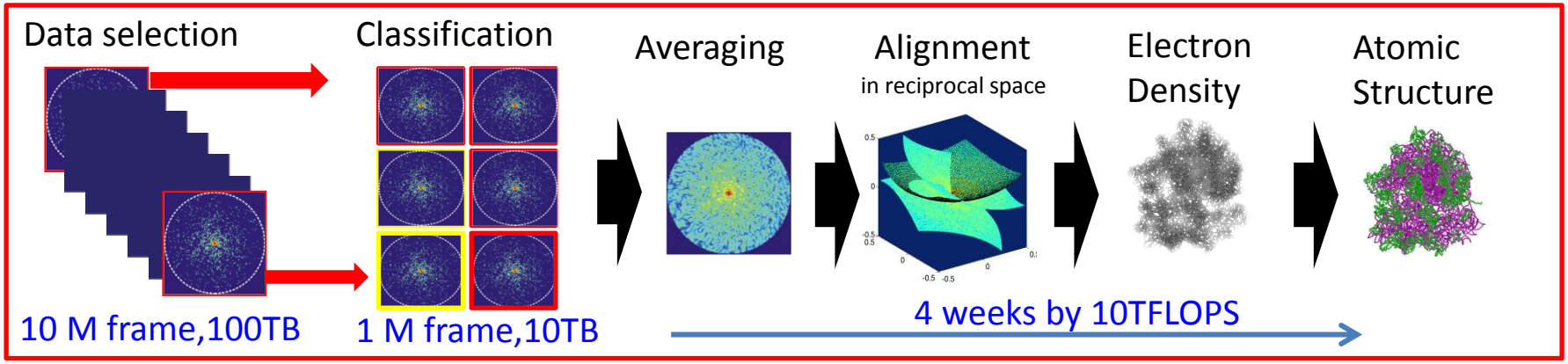
Full data analysis



Full Data Analysis (off-line)

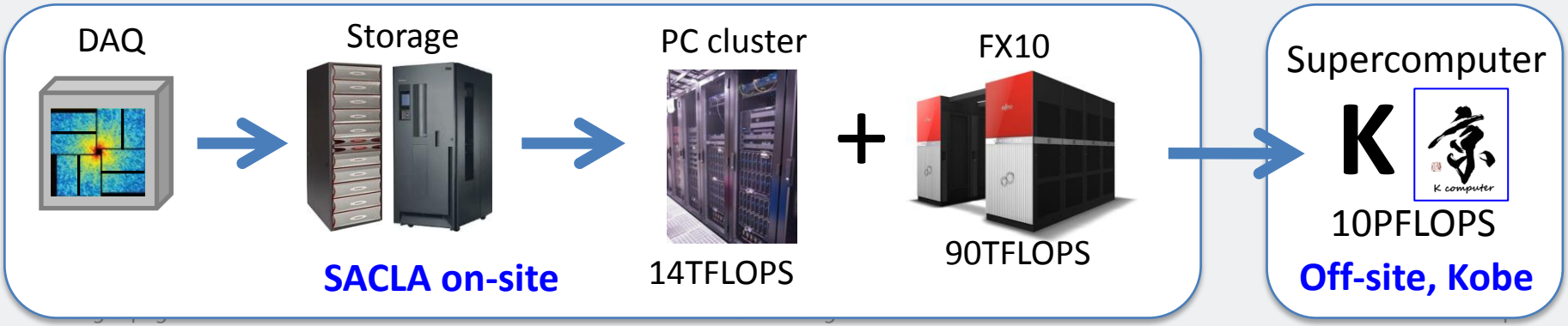
- data selection using low-level filtering
- classification
- averaging
- alignment
- reconstruction of 3-D image

Full data analysis scheme



- Big data processing is indispensable for 3D analysis
  - 10^6 frames for analysis ⇒ 10^7 frames for data taking (including junk).
  - 4 days data taking at 60Hz ~ 100TB storage size.
- Estimated CPU time for phase retrieval to get the atomic structure
  - 4 weeks by 10 TFLOPS PC cluster.
  - 3 days by 100 TFLOPS supercomputer.

-> Experimentalist requires more computing power.

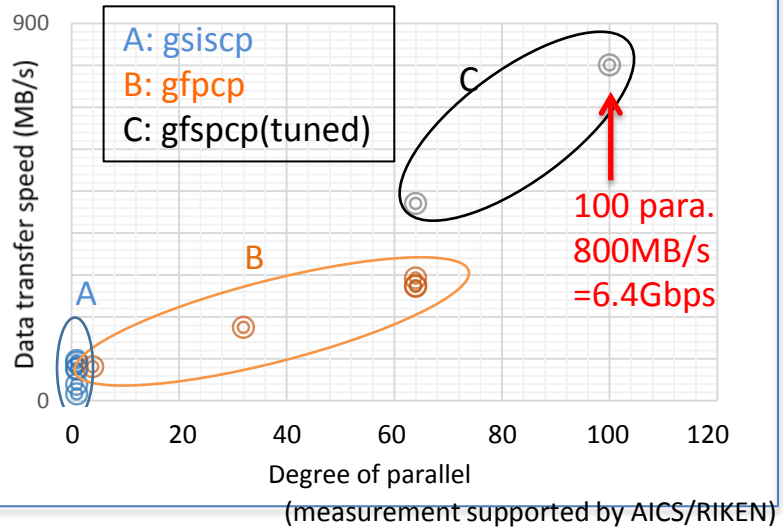


Data analysis plan using supercomputer 'K computer'

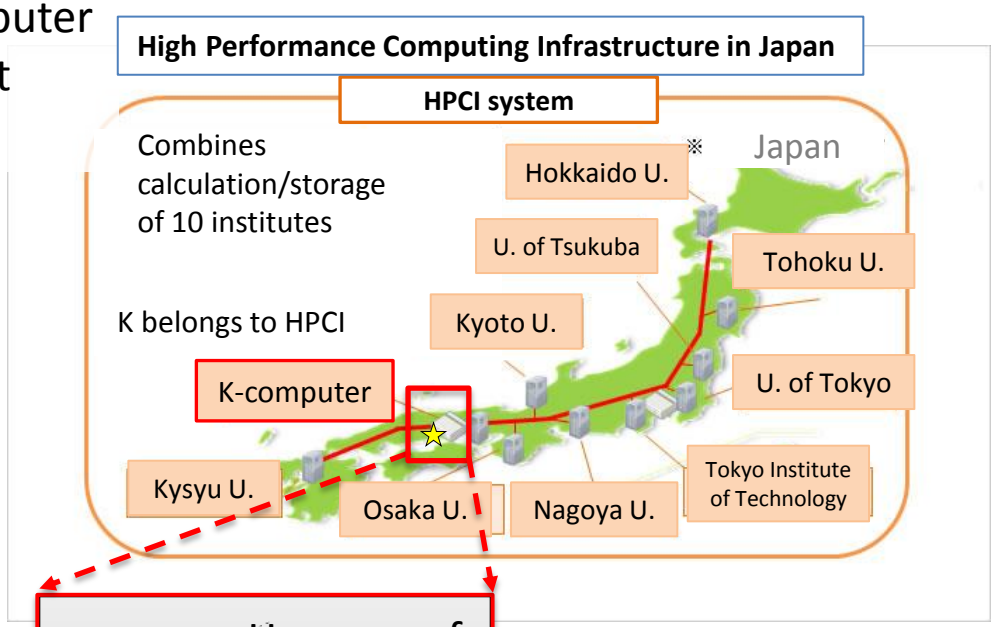
We just started feasibility study to use K computer for not only full data analysis, but also prompt data analysis.

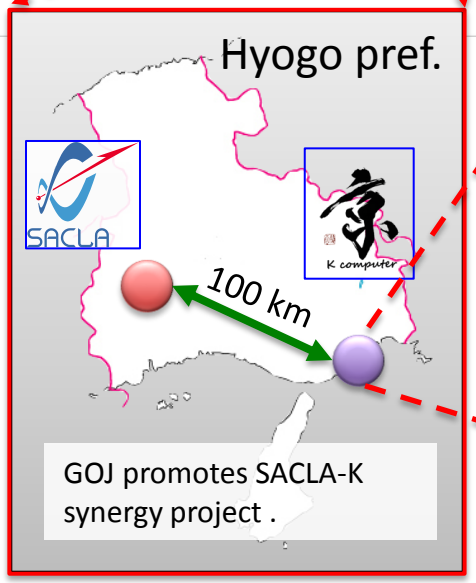
SACLA-K synergy

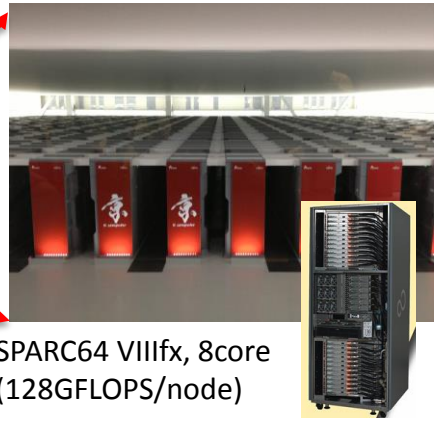
1. We carried out a preliminary data-transfer and job submit from SACLA to K computer.
2. We achieved 6.4Gbps bandwidth, which satisfy the experimental data rate.



(measurement supported by AICS/RIKEN)







SPARC64 VIIIfx, 8core (128GFLOPS/node)

Summary

- SACLA provides new opportunity to study complex targets using XFEL, especially, reveal 3-D structure of proteins.

- We developed DAQ and Analysis system for SACLA to satisfy experimental requirements:
  - 6 Gbps data rate
  - 120 TBytes data storage per protein sample
  - short experimental period (a few days cycle)
  - high computing power
    - 10 TFLOPS for run-by-run prompt analysis
    - 100 TFLOPS for full data analysis

    ... and more computing power!

- We also started feasibility study of joint analysis using K computer, which is 10 PF supercomputer at Kobe.

SACLA

backup