

HEPS Data Service System

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on behalf of HEPS CC group

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Overview

- 战略研讨会：希望HEPS做到科学实验过程和数据处理自动化....
- 暂时纯粹从需求出发的设计，侧重于功能性设计
- 希望做到“大”IT的框架设计
 - 用户视角：用户实验全过程的信息化、自动化、便利化
 - 设施运行视角：设施运行的数据化/数字化、尽可能的自动化，高效、可靠、协同
 - IT任务视角：软硬件架构和功能模块化，功能丰富、接口及数据标准化；数据格式标准化；综合服务服务化；

HEPS

- High Energy Phonon Source (HEPS)
- An major Infrastructure project of 13th Five-Year Plan
- The most brilliant source worldwide
- High energy, low emittance
- Investment of 5 billion RMB
- Construction started from Jul. 2019, operation expected in 2025

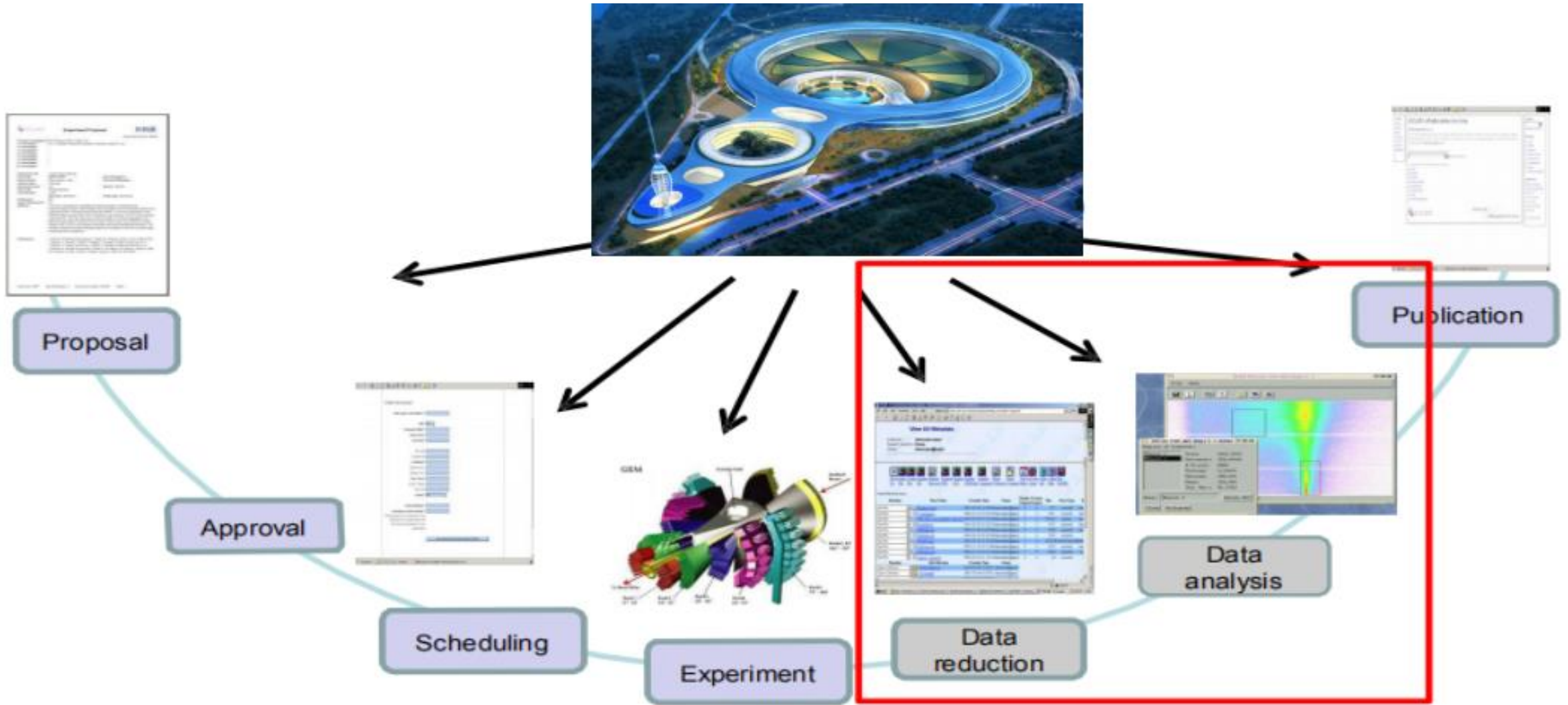


Table: Estimated data rates of HEPS beamlines.

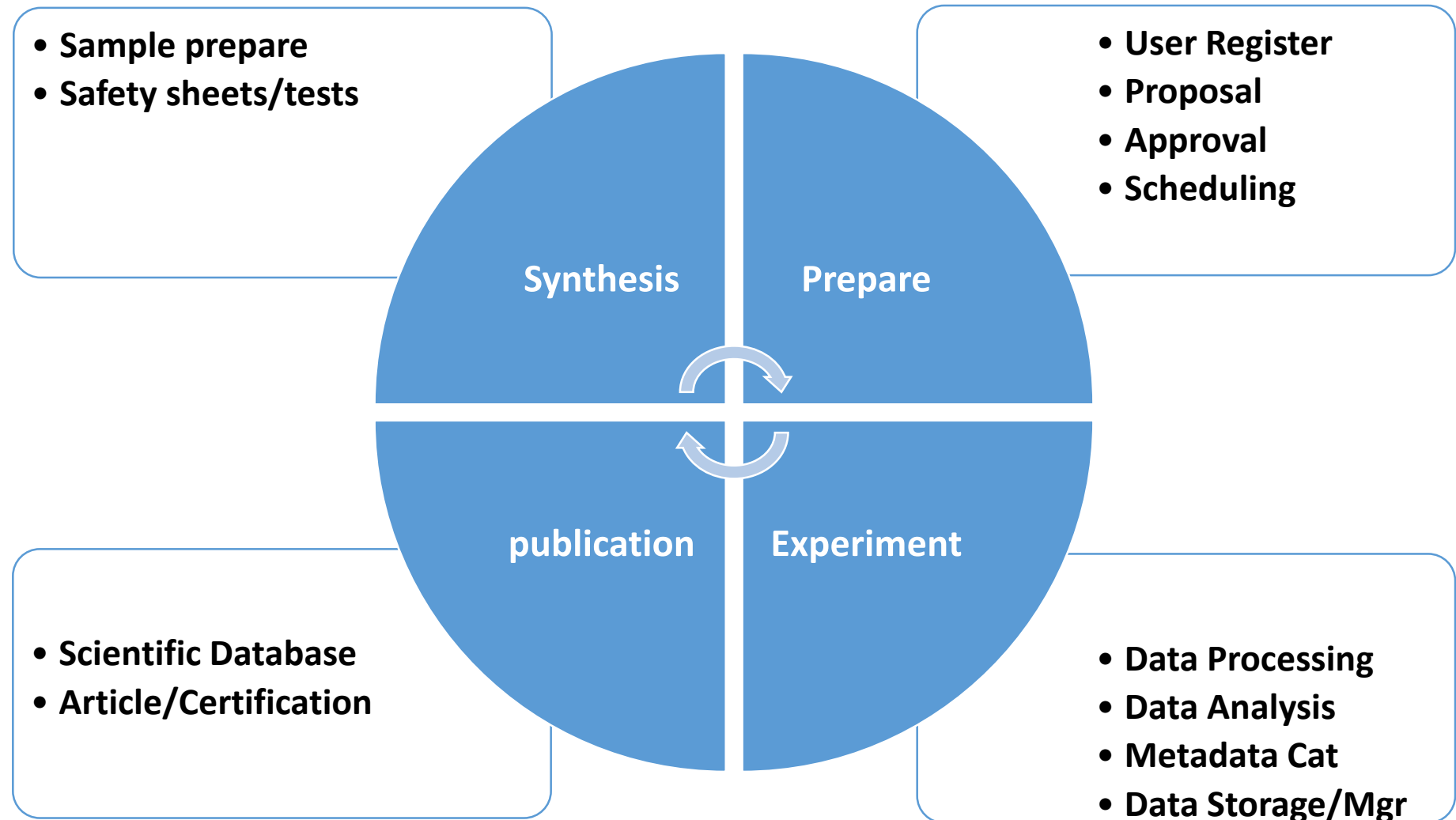
Beamline	Average output (Byte/day)	MAX burst (Byte/day)
B1	820G	4T
B2	14T	20T
B3	112.5G	1.4T
B4	2T	2T
B5	6.8G	10G
B6	20G	50G
B7	95T	520T
B8	10.32G	30G
B9	5G	10G
BA	35T	35T
BB	91.08G	165.6G
BC	1T	1T
BD	275M	500M
BE	11.2T	25T
TOTAL	159.27T	608.67T

Beamline	Bandwidth demanded
B1	40Gbps
B2	100Gbps
B3	1Gbps
B4	40Gbps
B5	1Gbps
B6	10Gbps
B7	100Gbps
B8	100Mbps
B9	100Gbps
BA	10Gbps
BB	100Mbps
BC	10Gbps
BD	1Gbps
BE	40Gbps
TOTAL	553.1Gbps

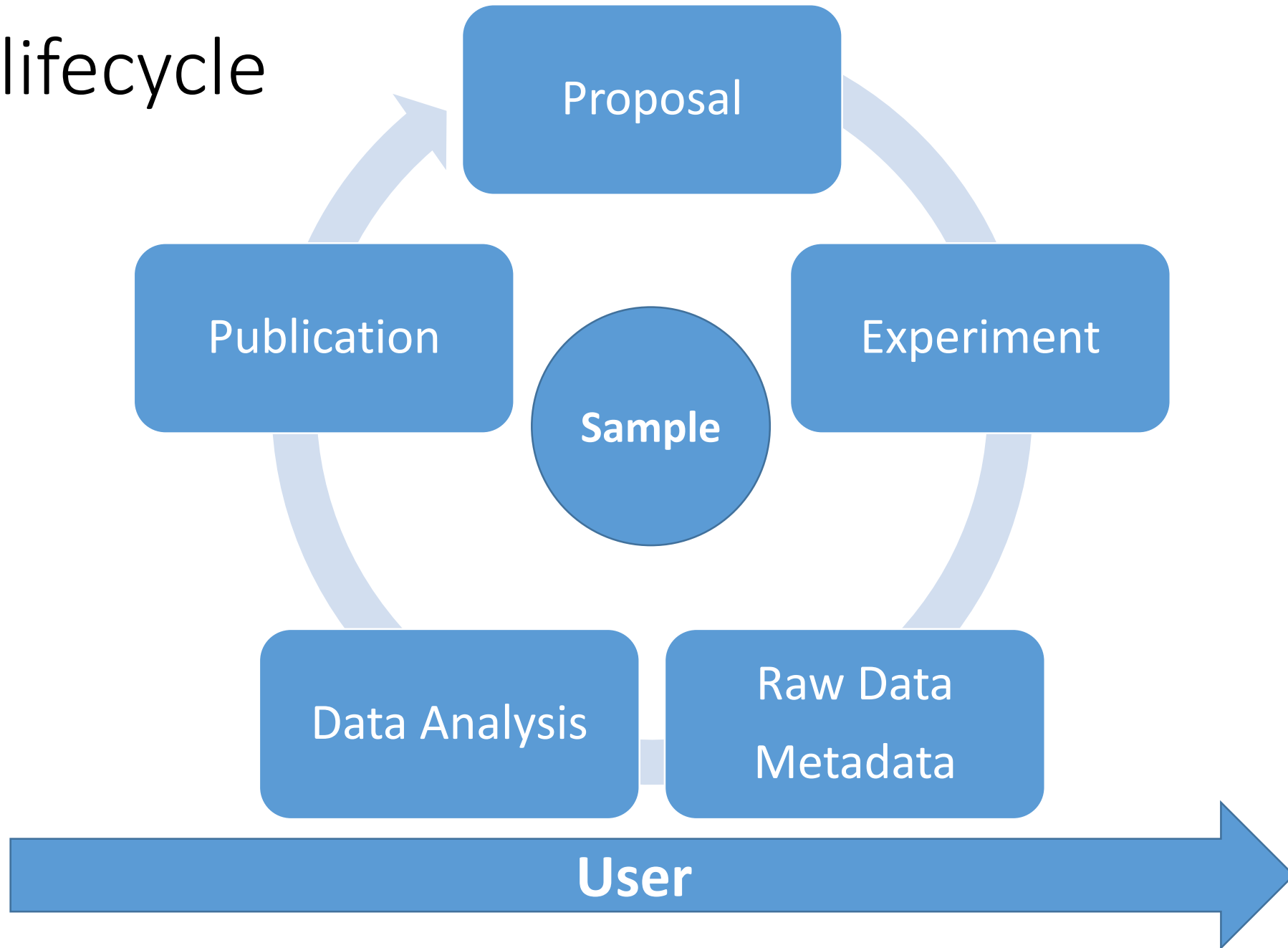
Beamline	Data format
B1	tiff
B2	hdf5
B3	tiff、SIF、dat
B4	hdf5
B5	hdf5、spec、mca、tiff
B6	tiff、hdf5
B7	
B8	txt、mca
B9	txt、tiff
BA	hdf5
BB	tiff
BC	pxt
BD	hdf5、mca、txt
BE	binary和tiff
TOTAL	Tiff、SIF、dat、mca、pxt、hdf5、spec、binary

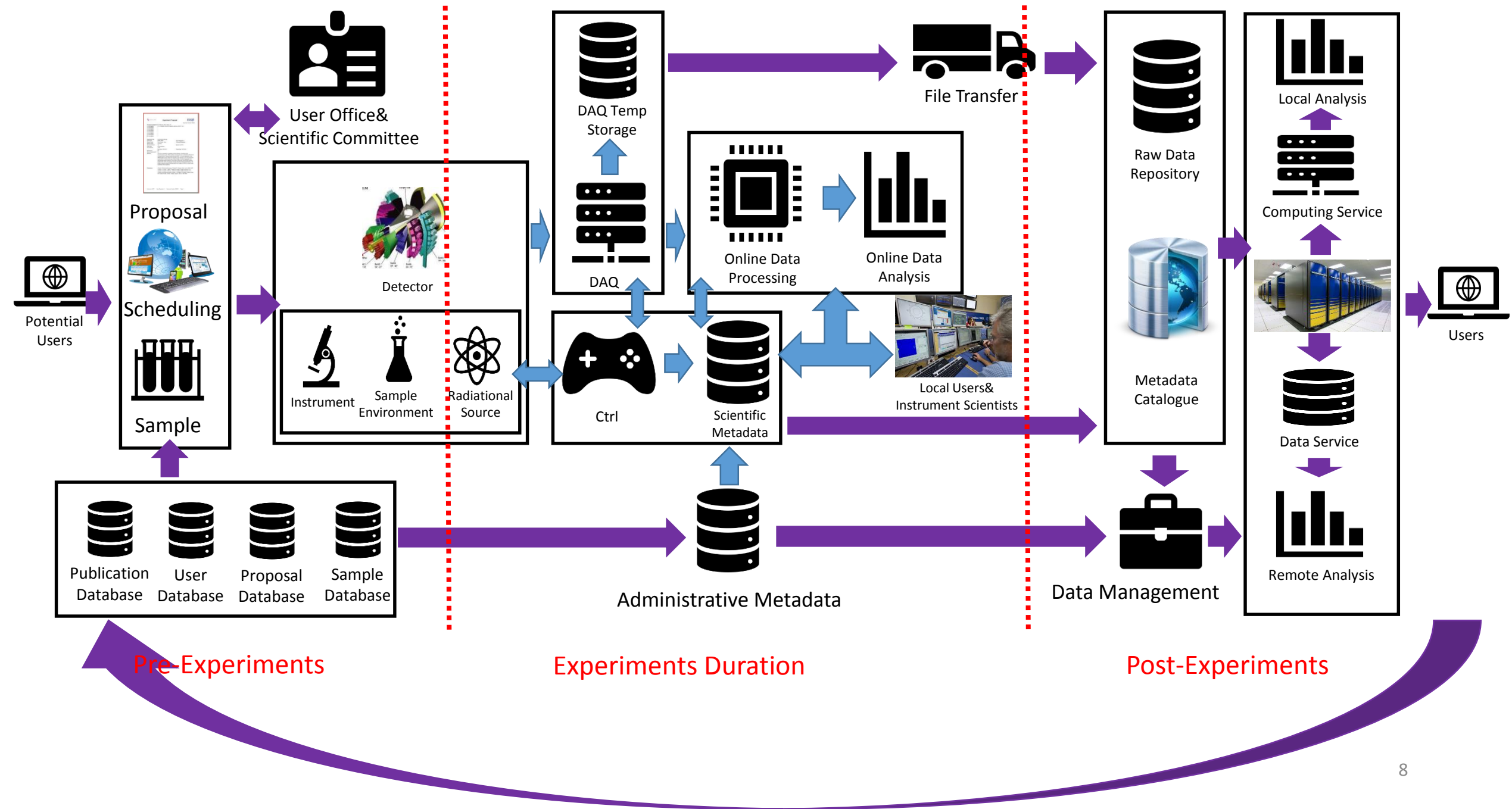


Research (user view)



Data lifecycle





Facility Management System

- ✓ Facility Database
- ✓ Facility Operation & Monitoring System

User Service System

- ✓ User Database
- ✓ User Safety Training System
- ✓ Proposal System
- ✓ Sample Management System
- ✓ Single-Sign-On
- ✓ Import proposal details from user portal: Experiments, samples details, etc.
- ✓ Create users, groups and setup permissions
- ✓ Create folders structure for storing scientific data

Data acquisition layer

- ✓ Set of data aggregator running on cluster of high-performance computers
- ✓ Collect, monitor and store experiment data
- ✓ Disseminate data to online cache and analysis pipeline

Run management service

- ✓ Coordinates PC layer activities related to data

Metadata catalogue (MDC)

- ✓ Organize and keep track of experiment data in a homogeneous and consistent way

Control Layer

- ✓

Accelerator & Beamline Optimization

- ✓ Running & Operation Log Collection and Analysis
- ✓ Feedback to Facility

Data management online -> offline

During measurement (run)

- ✓ Calibrated and raw data available in hutch (GUI, online)

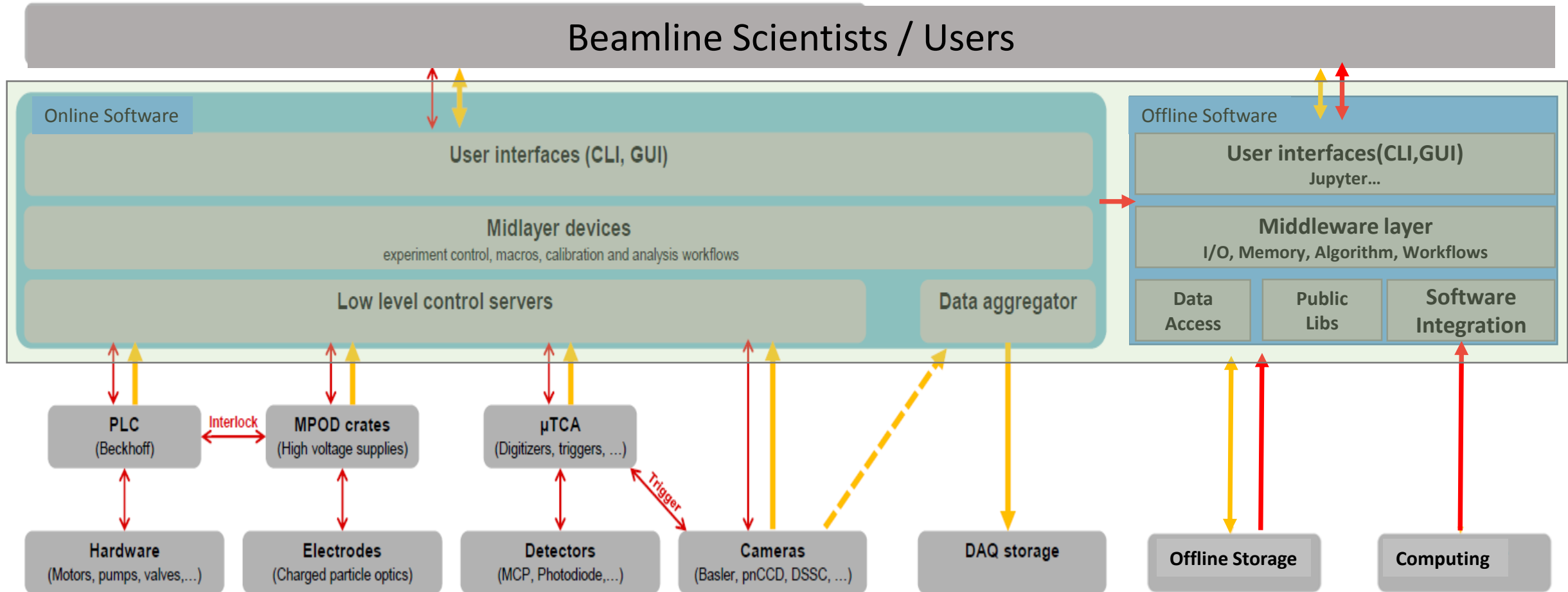
Data migration after each run

- ✓ Data manager decides on quality of the data: "good", "unclear", "not interesting" "good" and "unclear" data transferred to "Offline cluster"
- ✓ Migration triggers computation of calibrated data at online cluster

Post experiment

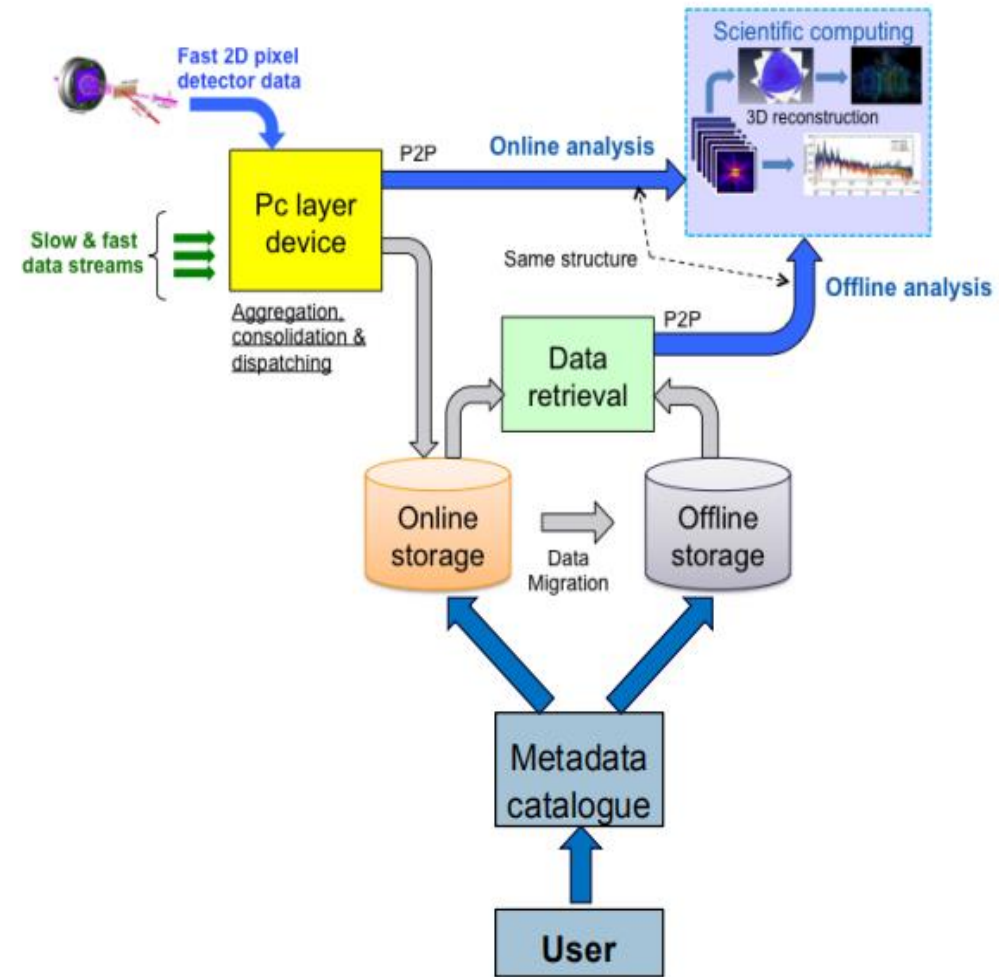
- ✓ Raw and calibrated data is available
- ✓ Data catalog is available
- ✓ Data service is available for search, access, download, interface to remote analysis
- ✓ Analysis resources / "Offline cluster"

Core Software



HEPS Data Policy (Refer to Eur.-XFEL)

- Raw data and metadata is stored, curated, and archived by HEPS
- Access to data through searchable metadata catalogue
- **Raw and metadata will be open access after embargo period**
- Electronic logbook will be provided for documentation
- Access to metadata catalogue and computing infrastructure through HEPS user account
- Online analysis and offline analysis should be provided
- Related system
 - Control / DAQ / Offline / ... /User Office



Control and Data taking

• Setup

- Retrieve experiment and sample metadata for the given proposal
- Receive and process run configuration
- Dispatch this metadata to Aggregators

• Data taking

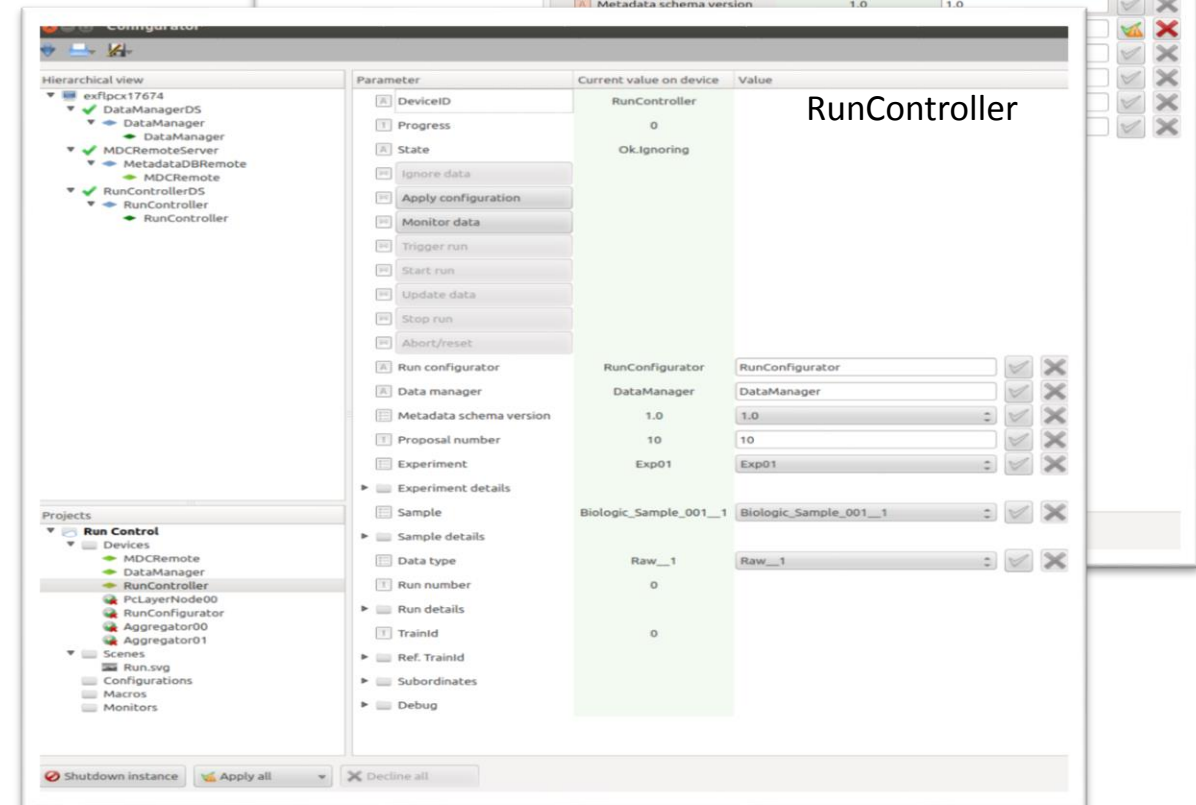
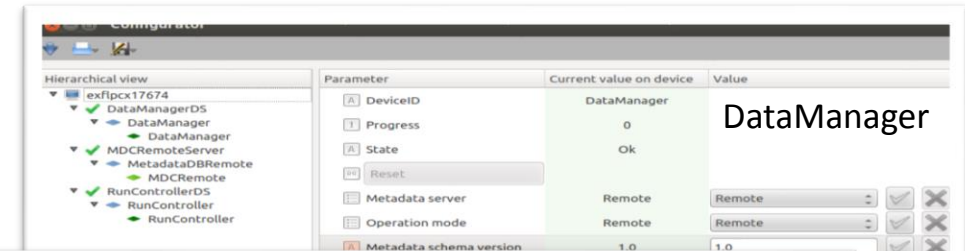
- Instruct start and stop of runs

• Publish data

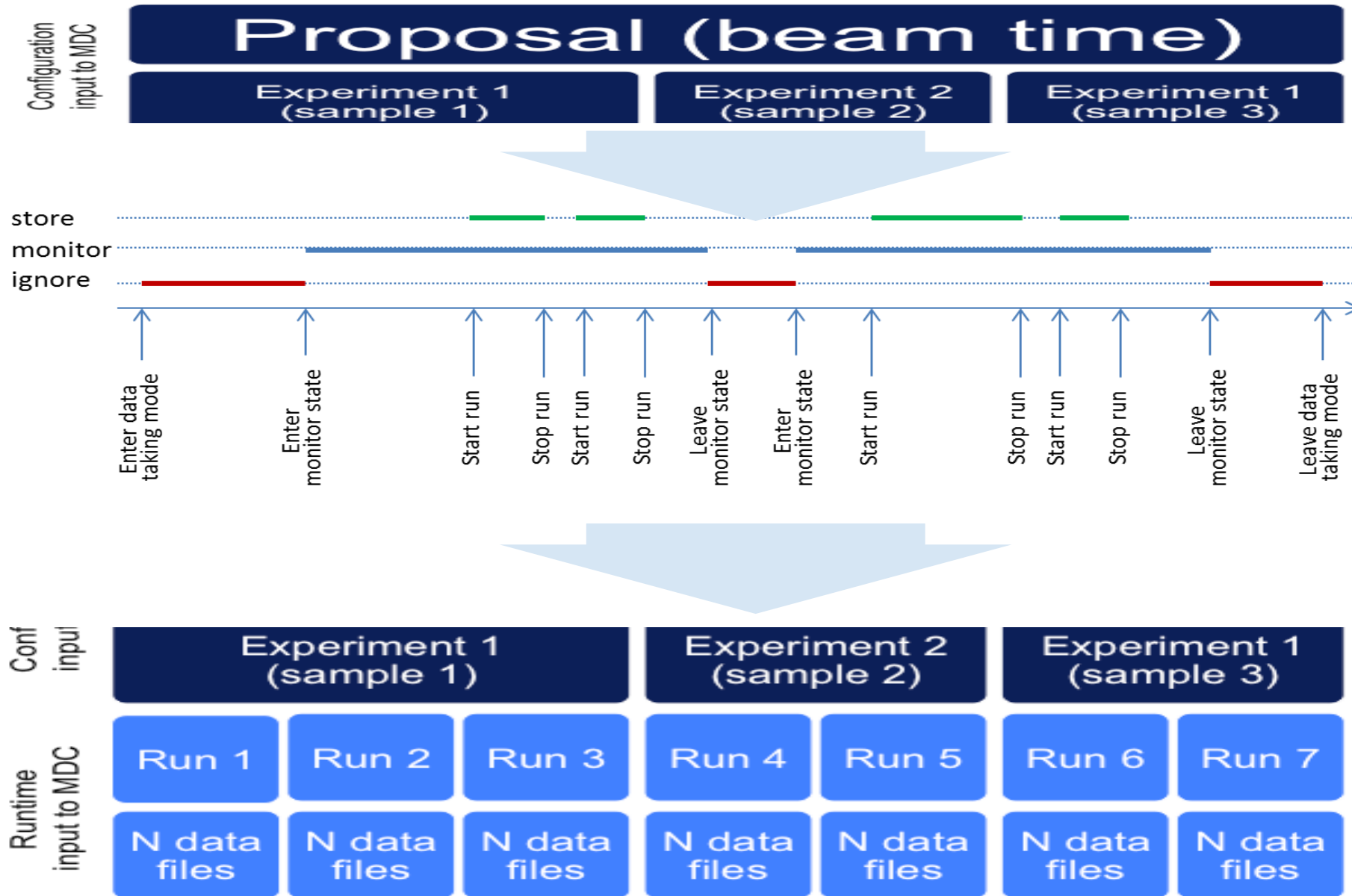
- Build run summary and register data files

New setup/experiment

New run



Scientific data collection/DAQ



User submit/edit proposal



User performing experiment (timeline)

Logical structure of experiment and runs

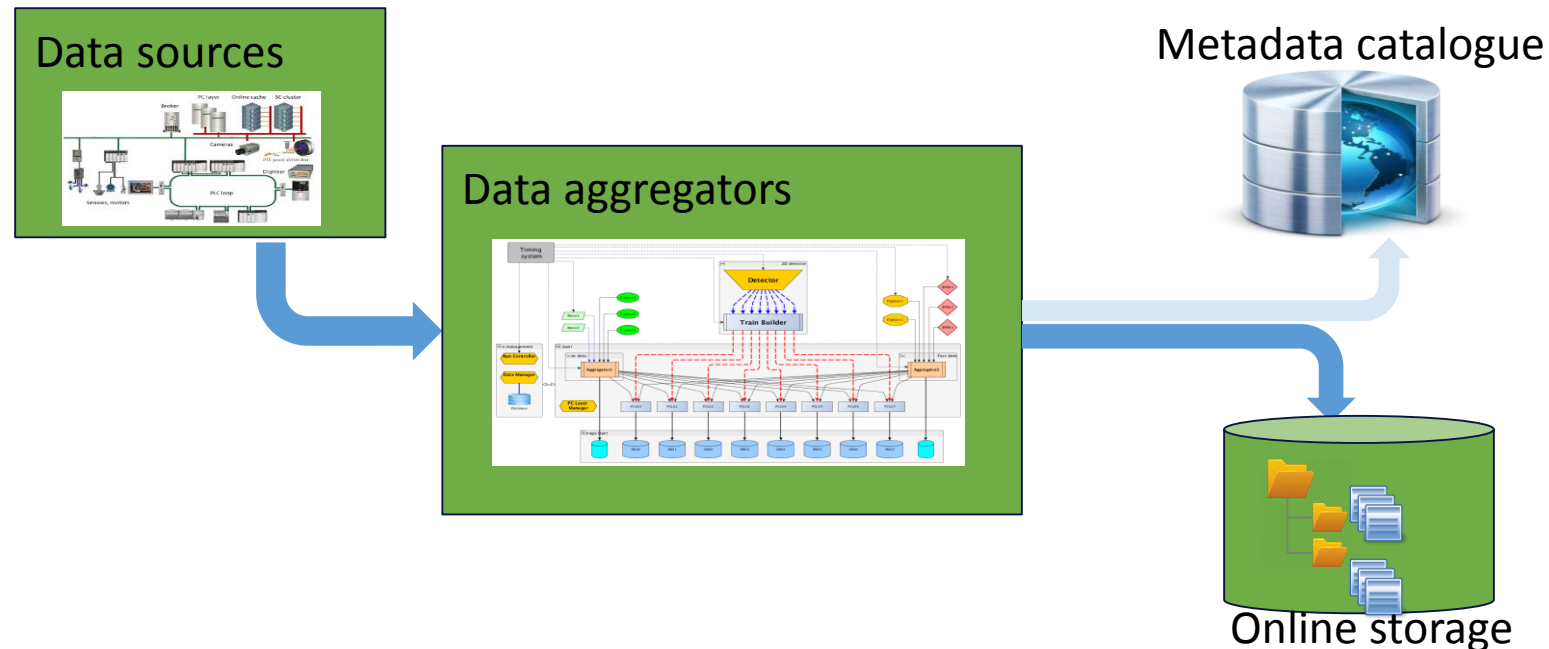
Data aggregators

- Functions

- Correctly receiving data from fast and slow sources
- Consolidating data streams from all data sources
- Monitoring, fast-feedback analysis, rejection and reduction
- Formatting and recording to HDF5 data files
- Data formats for FPGA binary, Control and Instrument data

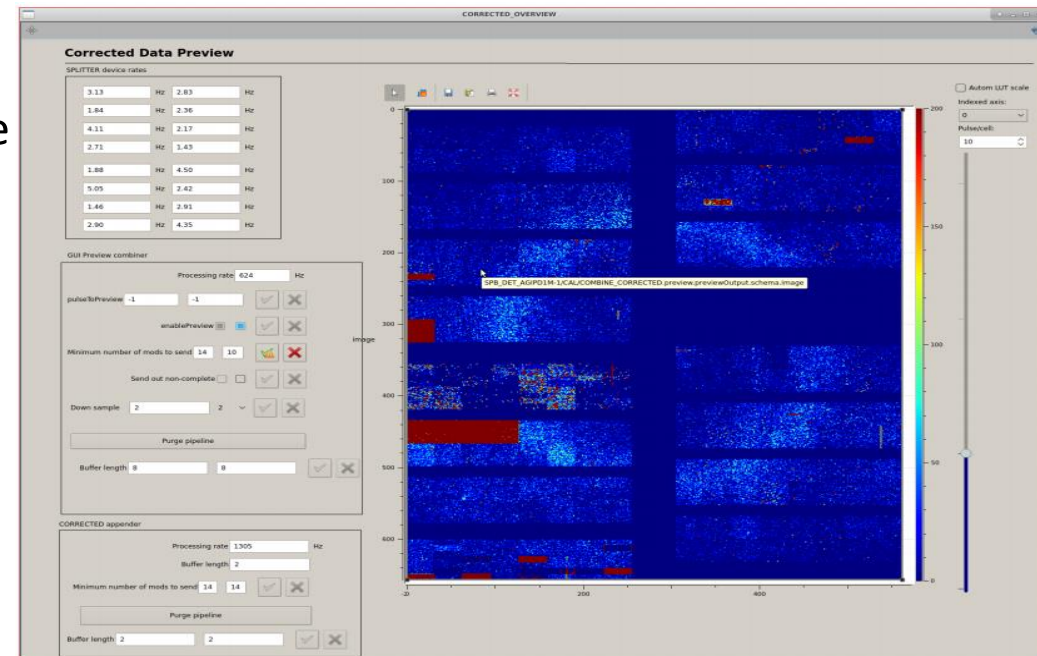
- Inputs and outputs

- DAQ/ Control/ User system
- Rawdata / Metadata catalogue



DAQ & Online Analysis

- FPGA / CPU / GPU based
- Distributed Resources
 - Storage and computing
 - Locates in beamline
 - Central management for infrastructure and public software
 - User defined application software
- Central Resources
 - Locates in Computer-Center
 - Virtualization for beamlines
 - Central management for infrastructure and public software
 - User defined application software
- Interfaces
 - Common data interface with analysis algorithms
- Rapid feedback through GUI
 - Scientific data
 - Control data
 - Facility operation logs
 -

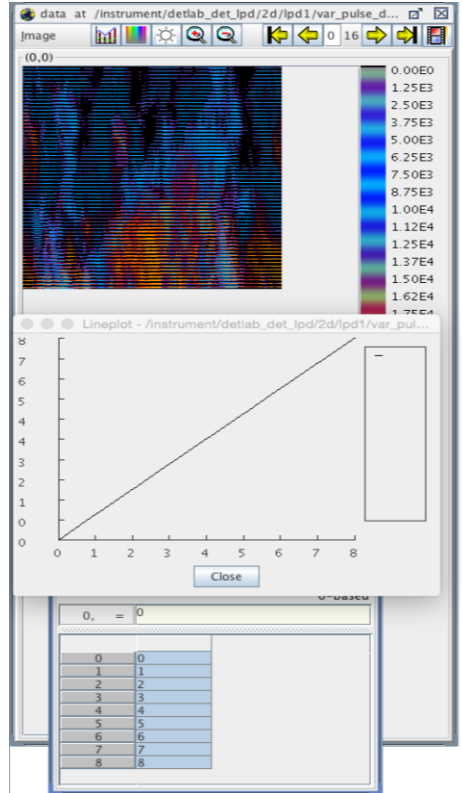


Data Services

Run number	Experiment	Sample	Start date	End at	First train	Last train	Available	Fig status	...
1373474128	Exp01 djellou_dev	Biologic Sample 002	May 18, 2016 15:36	-	120	200	✓	1	...
253398910	Exp01 djellou_dev	Biologic Sample 002	May 18, 2016 15:35	-	120	200	✓	1	...
1136444119	Exp01 djellou_dev	Biologic Sample 002	May 18, 2016 15:35	-	120	200	✓	1	...
1422343480	Exp01 djellou_dev	Biologic Sample 002	May 17, 2016 16:50	-	120	200	✓	1	...
858038635	Exp01 djellou_dev	Biologic Sample 001	May 25, 2016 00:00	-	159	263	✓	1	...
1785653778	Exp01 djellou_dev	Biologic Sample 001	May 25, 2016 00:00	-	159	263	✓	1	...
761474139	Exp01 djellou_dev	Biologic Sample 001	May 25, 2016 00:00	-	159	263	✓	1	...
1219146162	Exp01 djellou_dev	Biologic Sample 001	May 25, 2016 00:00	-	159	263	✓	1	...
1316274046	Exp01 djellou_dev	Biologic Sample 001	May 25, 2016 00:00	-	159	263	✓	1	...
2061843021	Exp01 djellou_dev	Biologic Sample 002	May 25, 2016 00:00	-	159	263	✓	1	...
1968369533	Exp01 djellou_dev	Biologic Sample 002	May 25, 2016 00:00	-	159	263	✓	1	...
201963407	Exp01 djellou_dev	Biologic Sample 002	May 25, 2016 00:00	-	159	263	✓	1	...
458122163	Exp01 djellou_dev	Biologic Sample 002	May 25, 2016 00:00	-	159	263	✓	1	...
222426879	Exp01 djellou_dev	Biologic Sample 002	May 25, 2016 00:00	-	159	263	✓	1	...
1016441043	Exp01 djellou_dev	Biologic Sample 002	May 25, 2016 00:00	-	159	263	✓	1	...
988031516	Exp01 djellou_dev	Biologic Sample 002	May 25, 2016 00:00	-	159	263	✓	1	...
1834719128	Exp01 djellou_dev	Biologic Sample 002	May 25, 2016 00:00	-	159	263	✓	1	...
1382743622	Exp01 djellou_dev	Biologic Sample 002	May 25, 2016 00:00	-	159	263	✓	1	...



List of files



Access data

Retrieve data

List of files

Reader

Facility	Type	Instrument	Instr. Cycle	BeamTime	Experiment Id	Run
HEPS	RAQ	B1	20190505	p000010	e0001	r0002

Local Access

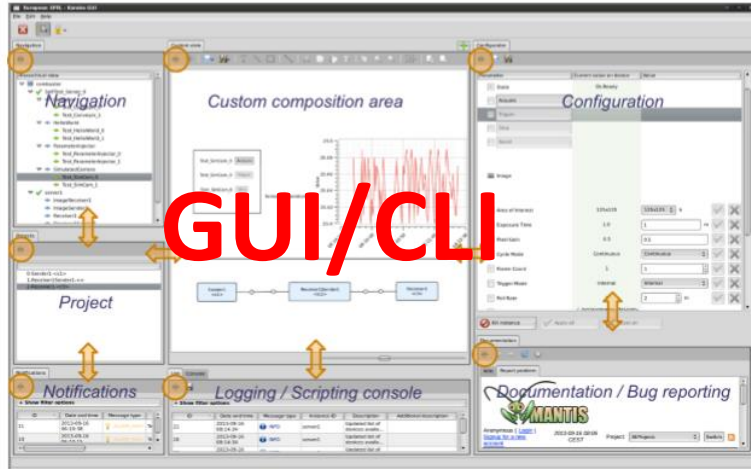


Remote Access

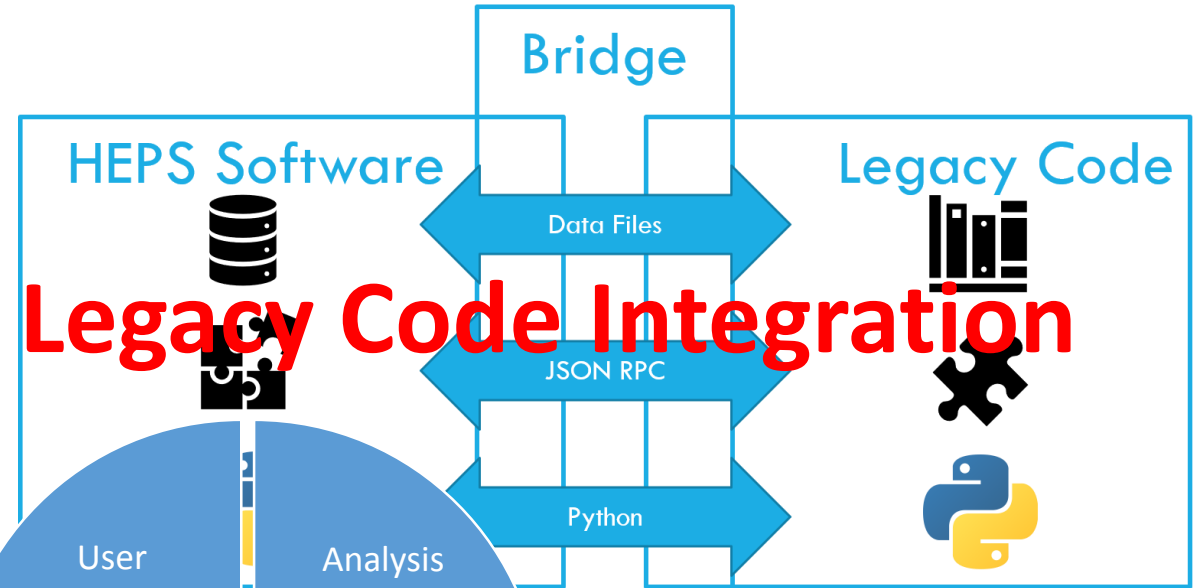


Key Technologies and Services

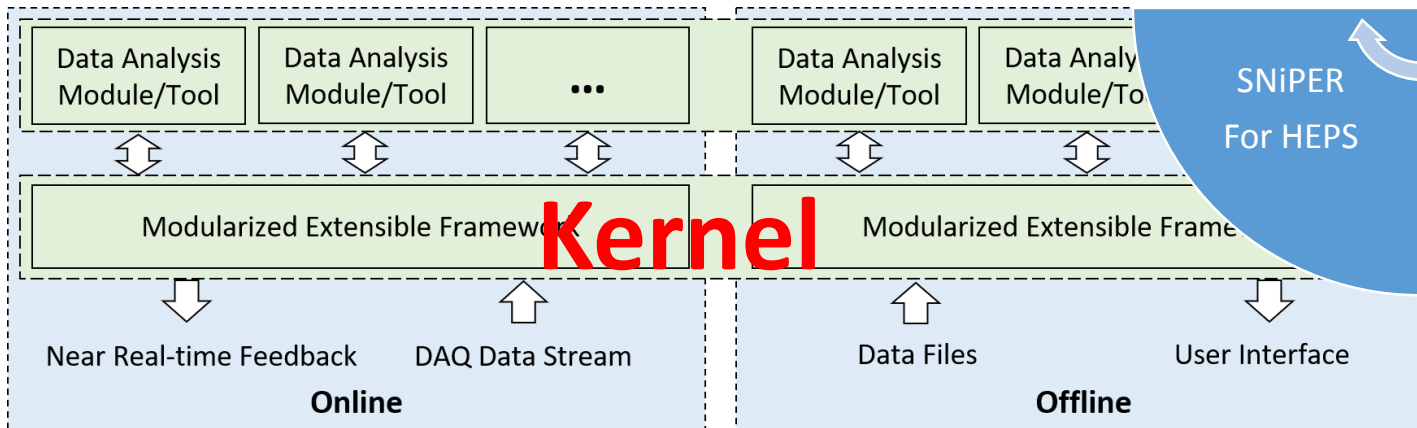
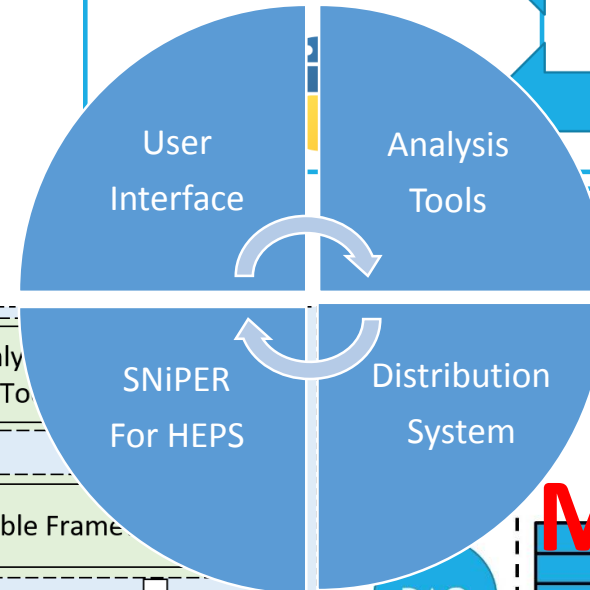
Software Framework



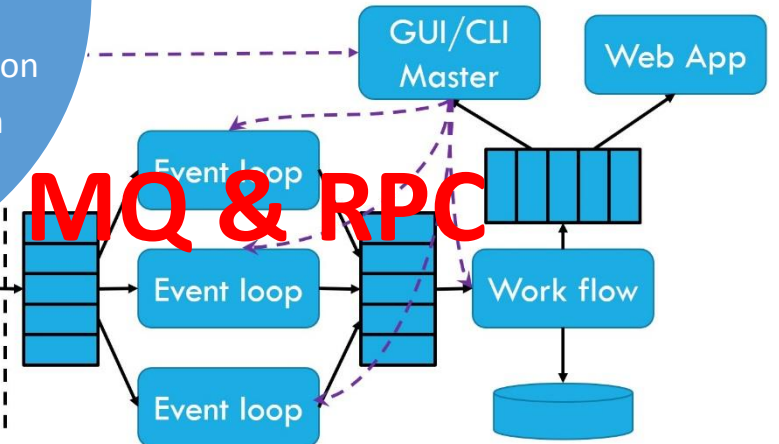
GUI/CLI



Legacy Code Integration

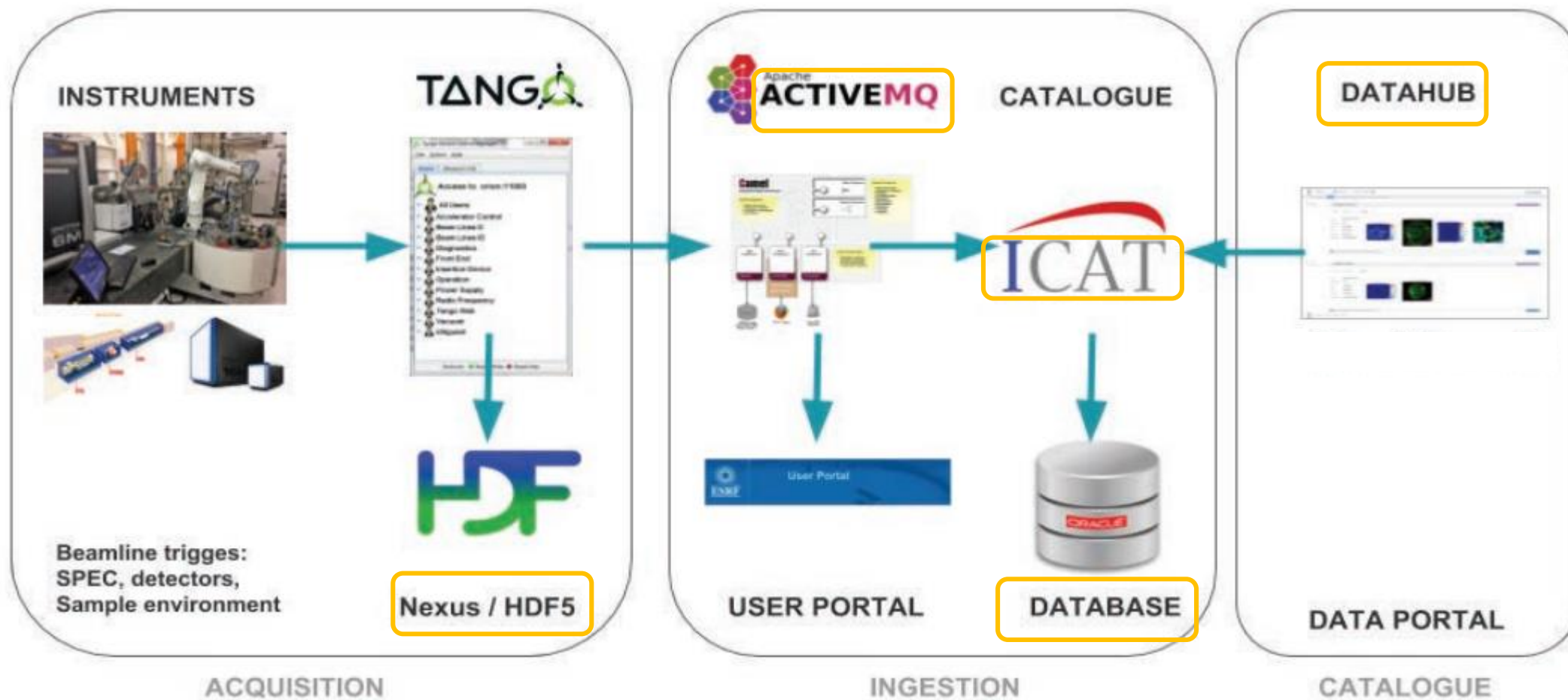


Kernel



MQ & RPC

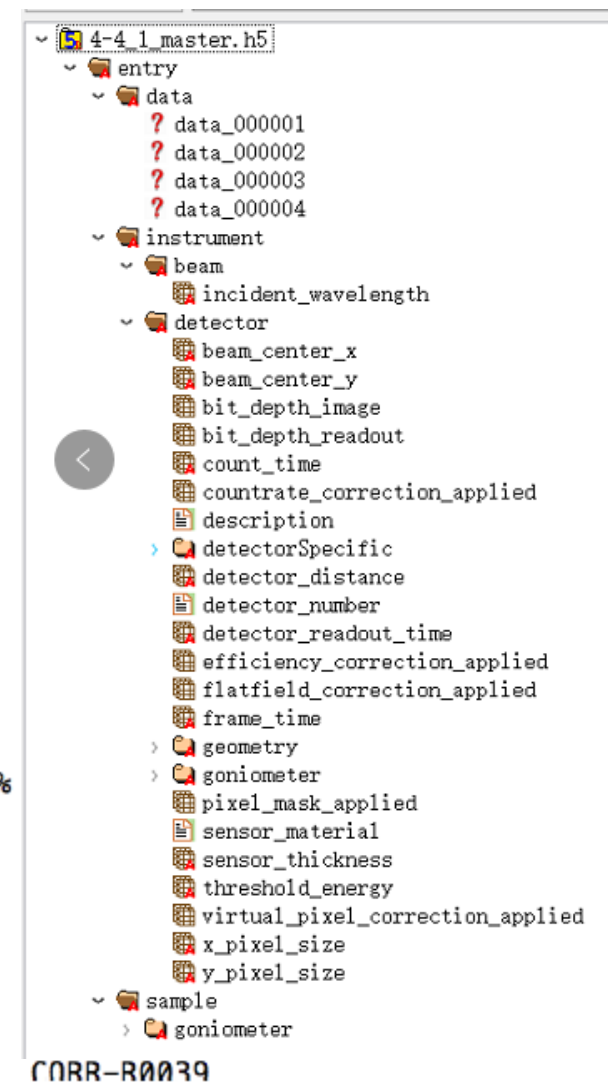
Data management



Raw Data Management / Raw Data Format

- Raw data: data files collected after each run
- Data format
 - HDF5: a file format for managing any kind of data
- Data format standardization
 - convert other data format (TIFF、SIF、MCA、TXT...) to HDF5
- Raw data repository:
 - File system storage
 - TIFF、SIF、MCA、TXT

```
[haufs@max-exfl014]/gpfs/exfel/exp/SPB/201701/p002038/proc%  
CORR-R0039-AGIPD00-S00000.h5 CORR-R0039-AGIPD05-S00002.h5  
CORR-R0039-AGIPD00-S00001.h5 CORR-R0039-AGIPD05-S00003.h5  
CORR-R0039-AGIPD00-S00002.h5 CORR-R0039-AGIPD06-S00000.h5  
CORR-R0039-AGIPD00-S00003.h5 CORR-R0039-AGIPD06-S00001.h5  
CORR-R0039-AGIPD01-S00000.h5 CORR-R0039-AGIPD06-S00002.h5  
CORR-R0039-AGIPD01-S00001.h5 CORR-R0039-AGIPD06-S00003.h5  
CORR-R0039-AGIPD01-S00002.h5 CORR-R0039-AGIPD07-S00000.h5  
CORR-R0039-AGIPD01-S00003.h5 CORR-R0039-AGIPD07-S00001.h5
```



Scientific Aggregators and Converter Module

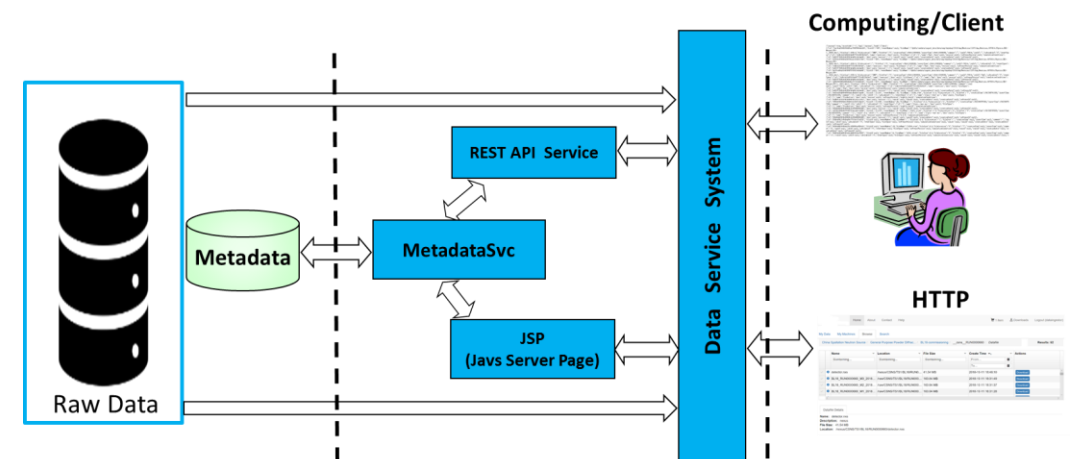
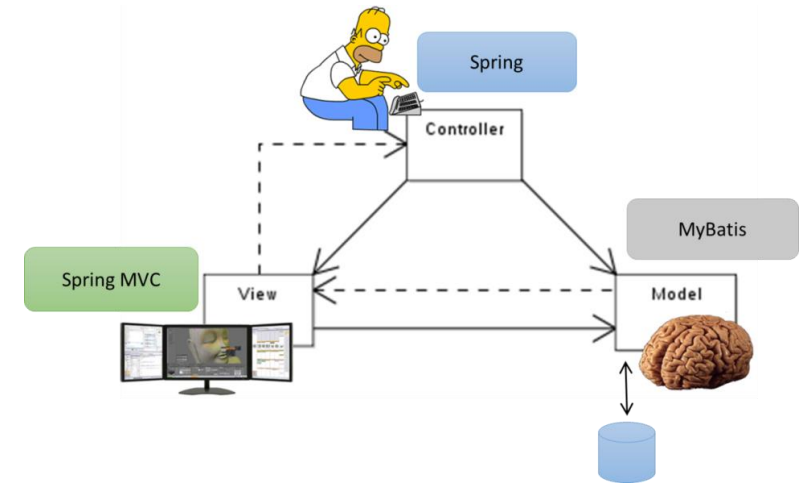
- Aggregation
 - raw data file + scientific metadata
 - Scientific metadata: sample, beamline and experiment parameters
- Conversion
 - to HDF5
- Control + DAQ + Offline

Metadata Management/ Data catalogue

- Meta data
 - administrative : data management lifecycle, ownership, filecatalog
 - scientific: describing the sample, beamline and experiment parameters relevant for the users data analysis
- Data model:
 - define common generic (fixed) meta data
 - allow completely flexible and rich structured (beamline, instrument specific) scientific meta data
- Storage
 - MongoDB backend
 - NoSQL -no fixed structure and common data format
 - Map/Reduce queries and the option to use JavaScript as the query language
 - Powerful indexing and support for file storage
 - Fault tolerant and drivers for most languages

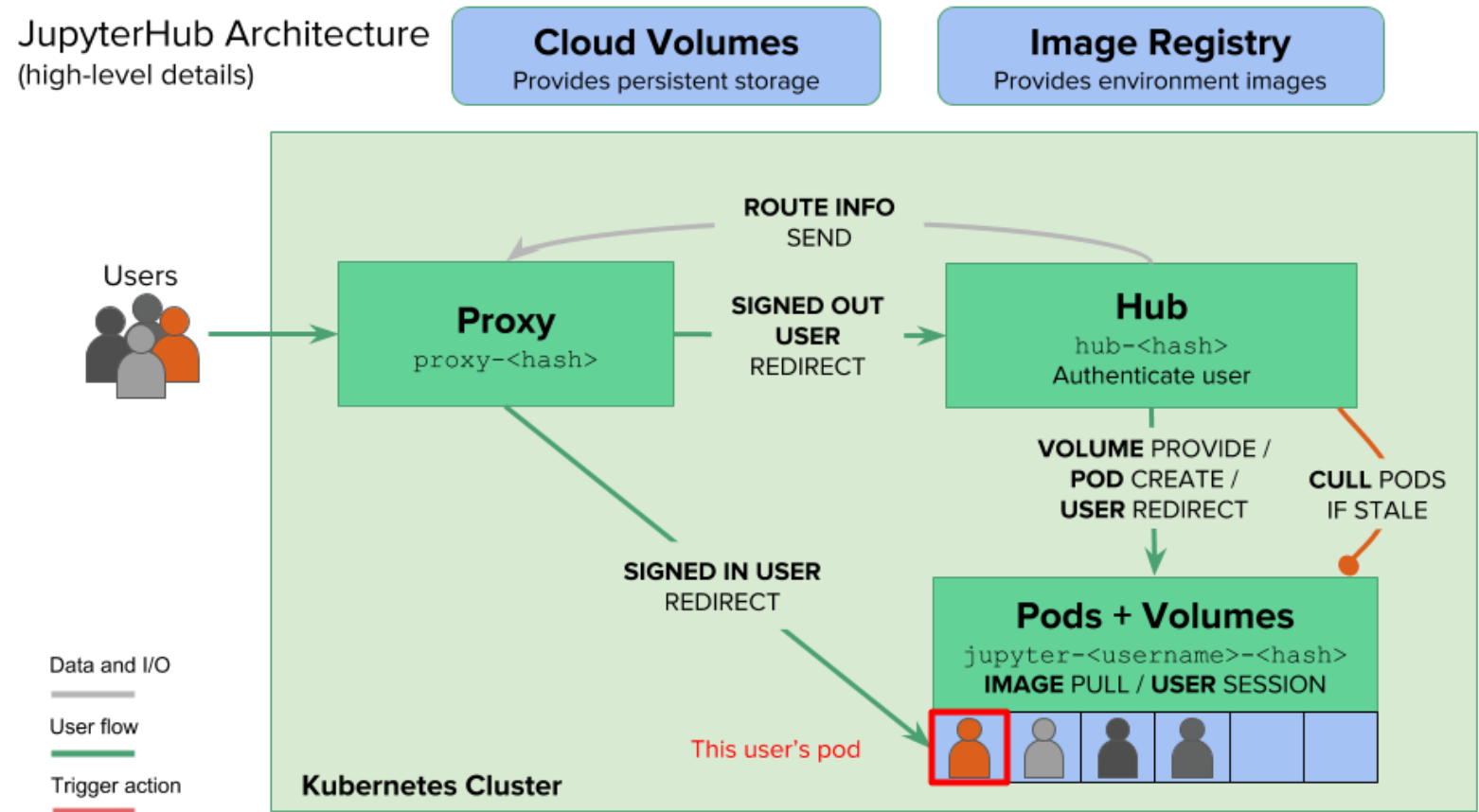
Data Service System

- Web based frontend
 - Find data based on the meta data
 - Download data based on data permissions
 - Data can be linked to proposals and samples
 - Data can be linked to publications
 - Helps keeping track of data provenance
- API Services
 - Computing: Local & Cloud
 - Client



Software –tools platform

- Gitlab/GitHub
- Matlab
- Ansys
- JupyterHub
-

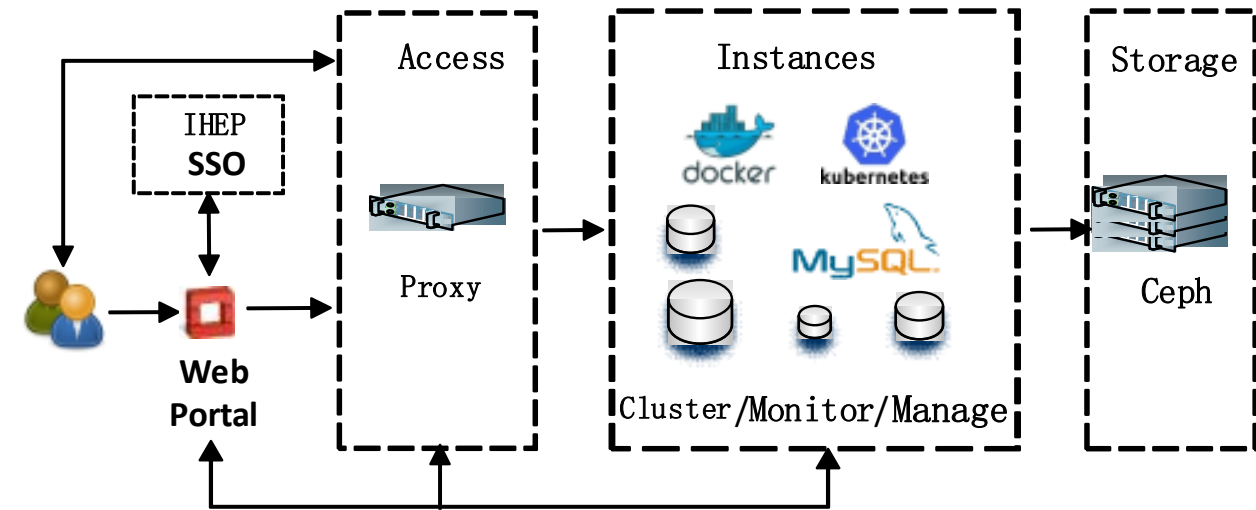


Database Services System

- Services for Database
 - Public databases
 - Facility Database
 - Operation Database
 - Scientific Database
- High performance and stability
- RD and NoSQL

No access to underlying hardware

No DBA support or application support



The screenshot shows the Lepus MySQL Resource Monitor dashboard. The interface includes a navigation menu on the left with options like Dashboard, Configure, MySQL Monitor, Health Monitor, Resource Monitor, Key Cache Monitor, InnoDB Monitor, TableSpace Analysis, Alarm Panel, and User Permission. The main content area displays the MySQL Resource Monitor with a search bar and a table of server connections.

Servers			Connections		
Host	Tags	Max Connections	Connected	max_connect_errors	open_files_limit
10.1.231.11:3306	master	3000	28	30	15000
10.1.231.12:3306	master	3000	2	30	15000
10.1.231.13:3306	slave	3000	1	30	15000

Facility Database

- 独立的固定资产管理
 - 采购、报销、入库、位置、状态
 - 属性管理
- 资产关系管理 (Relationship Management)
 - 父-子关系
 - 兄-弟关系
 - 树状结构
 - 举例：一个设备由多个部件构成，资产管理数据库能够反映出其部件组成关系及其关联的财、人关系



Facility Lifecycle Management

- 采购—报销—入库—上线—运行（巡检）—维修（升级）—下线—退库—报废



统计报表

灵活定制可视化图形报表，一键生成统计分析；
资产使用状态报表、资产分类报表、资产走势图；
多维度生成资产明细分析、汇总表，支持按条件导出；

全生命周期管理

跟踪资产启用直至资产退出，对整个资产全生命周期进行全程跟踪管理；

为管理者提供详实的资产数据汇总，可视化图形报表，管理变得更轻松；



资产盘点

盘点平台多样化，支持微信公众号、安卓平台、IOS平台以及WINDOWS工业平台采集设备和手机端APP；

可通过盘点计划、盘点批次、个人核查等多方式建立盘点任务；

盘点数据自动提交，快速自动生成盘点报表，实现多人同时参与盘点，高效提升工作效率；



采集设备



安卓平台



IOS平台



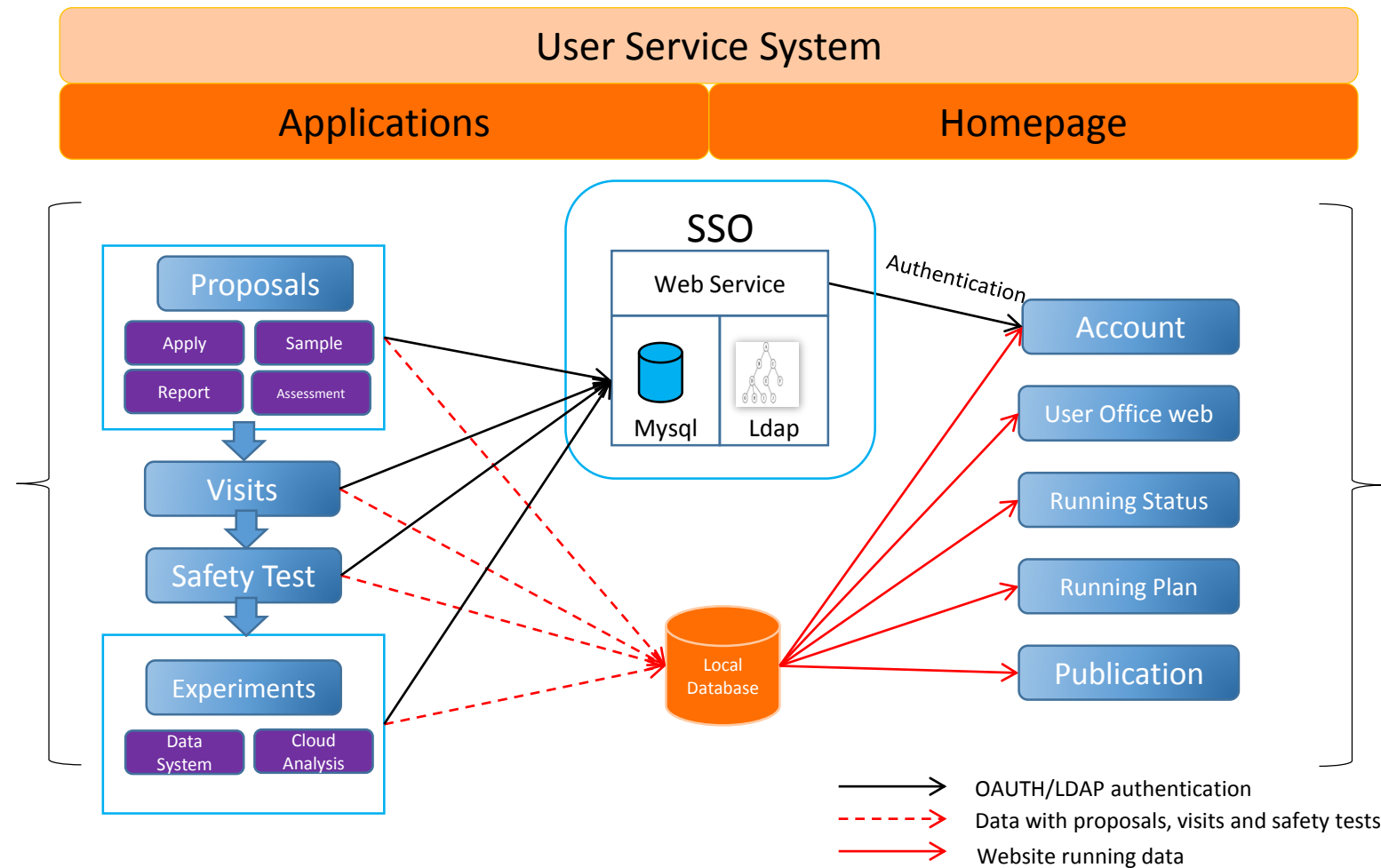
日常管理

资产入库、盘点、领用、变更、维修、调拨、报废清理等全生命周期管理；

告别传统的纸记手抄和Excel模式，全面进入无纸化资产管理方式；

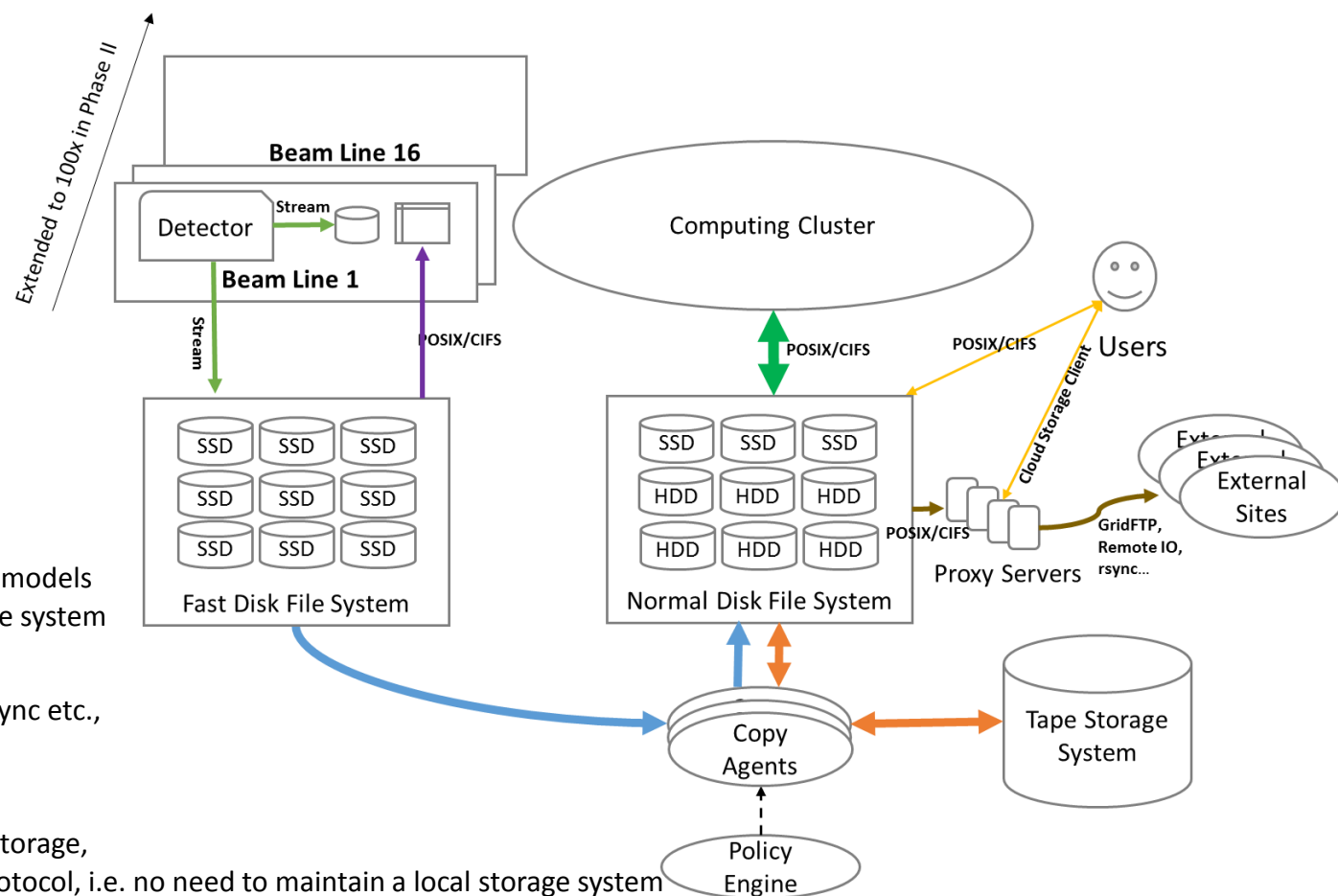
User & Proposal Service System

- One-stop Service System
 - Online experiment solution for scientists and students
 - One IHEP SSO Account for all services
- System Function
 - Proposals Application
 - Experimental risk assessment
 - Expert review
 - Safety Tests
 - Visits Arrangements
 - Running status statistics



Distributed / Central Storage Resources

- Fast Disk File System (managed by Lustre file system)
 - for fast on-line analysis, 10GB/s write, 20GB/s read
 - Sequential read and write, 1 day data life, 160TB Capacity
- Normal Disk Storage (managed by Lustre file system)
 - for batch jobs, interactive analysis, backups and data transfers
 - Mixed I/O patterns: sequential read and write, random read
 - 10GB/s write, 50 GB/s read, 6 month data life, 30 PB Capacity
- Tape Storage (managed by CERN CASTOR)
 - for data preservations and backups
 - Sequential Read and Write
 - 5 year data life, 300 PB Capacity
- Policy engine (developed by IHEP-CC)
 - make decision of data copies by static rules or prediction of AI models
 - scheduling and monitoring data copy requests between storage system
- Data transferring System (SPADE)
 - Transfers data to remote site before data analysis by gridFTP, rsync etc.,
 - multi-stream, presumable, schedulable transfers
- Data Federation (developed by IHEP-CC)
 - Users at remote sites can see an identical namespace of HEPs storage,
 - Remote sites can access data at HEPs storage by remote I/O protocol, i.e. no need to maintain a local storage system



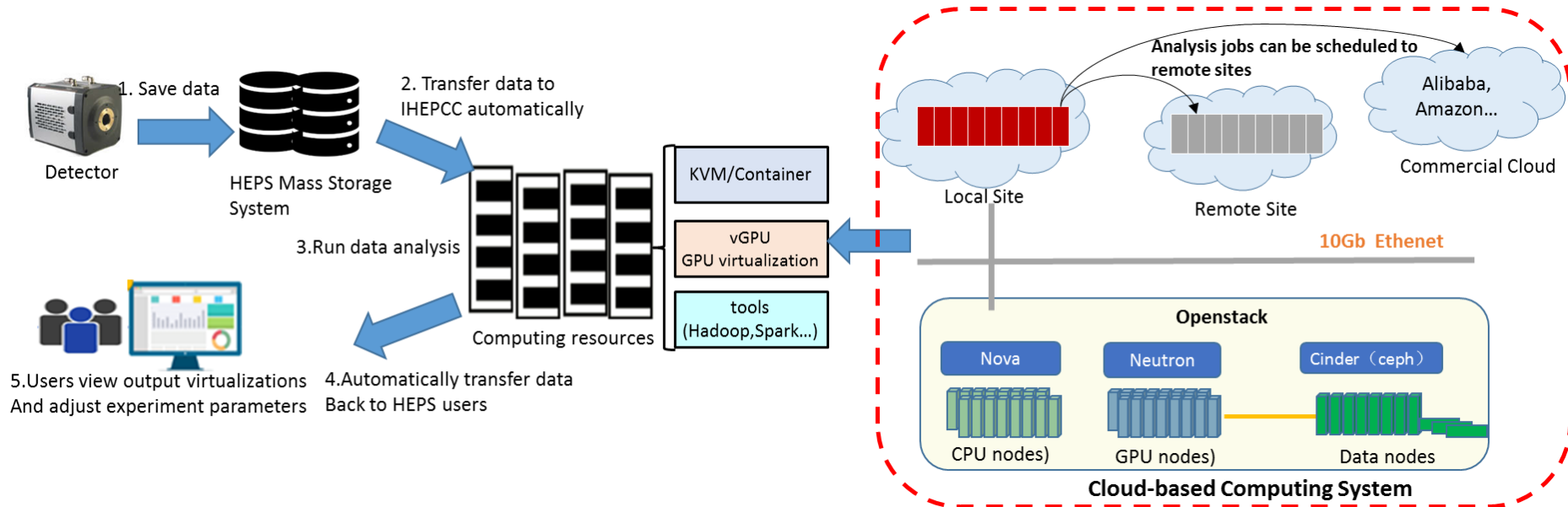
Distributed / Central Computing Resources

- **Cloud-based computing system**

- Deploy the various computing platform in cloud like batch farm, HPC farm and also develop with a rich collection of tools to work for Daas
- Integrate distributed computing resources as well as commercial clouds to expand computing scale based Openstack+HTCondor
- Using GPU virtualization technology to provide the HPC service in cloud
- Kubernetes+Docker to provide virtualized resources for WEB-based analysis

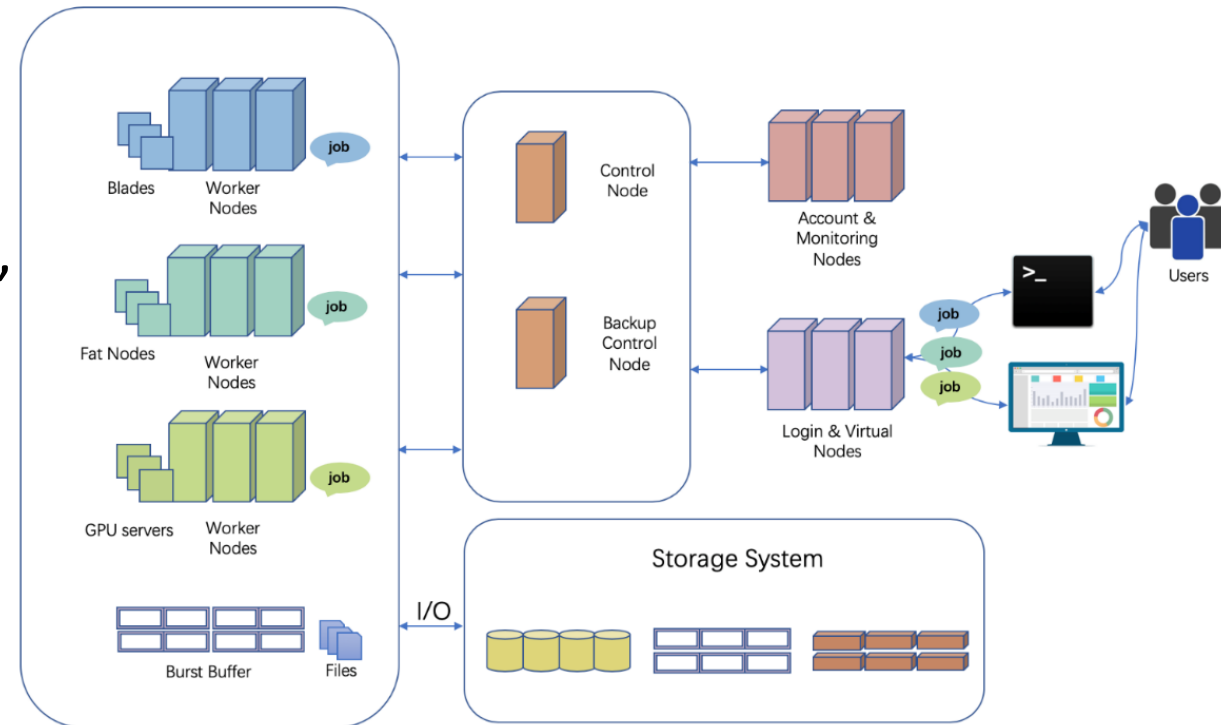
- **Requirements and Design**

- **Online data analysis(Streaming data services):** developed a rich collection of tools with the Hadoop and YARN including Spark for real-time analyzing streaming data after data acquisition
- **Offline Data analytics:** as implemented with the HEPS software to provide Data analysis as a service for users



High Performance Computing

- Flexible and elastic scale expansion design (designed by IHEPCC)
- Convenient and unified user job interface (developed by IHEPCC)
- Heterogeneous resources in cluster including CPU nodes, GPU nodes, fat nodes, with rich scheduling policies (Managed by Slurm)
- Various Operating systems and softwares provided to the job based container technology and transparent to user (developed by IHEPCC)
- Burst storage integrated with cluster providing high IO throughput during the job life time (Integrated by IHEPCC)



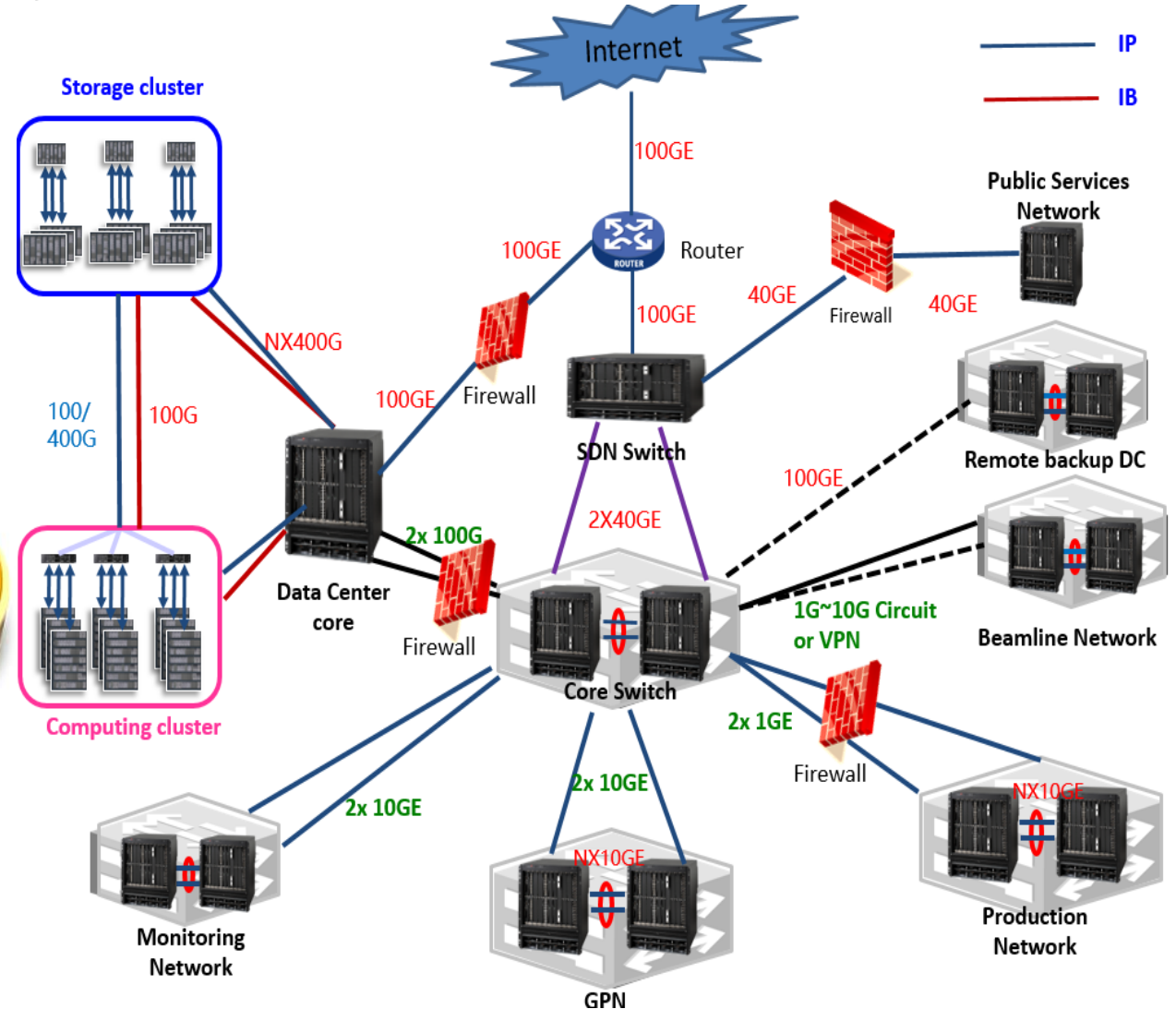
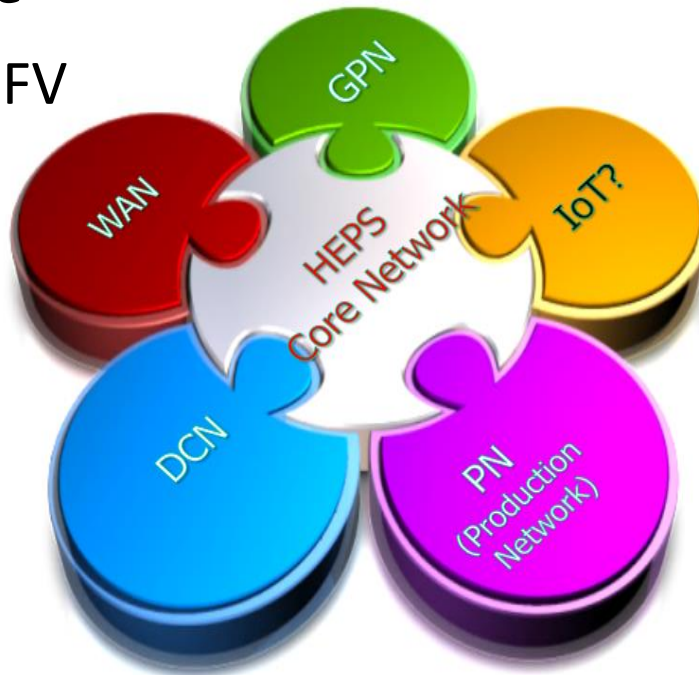
ML Platform

- For Scientific Data Analysis
- For Facility Operation Log Analysis
-

Network and Security

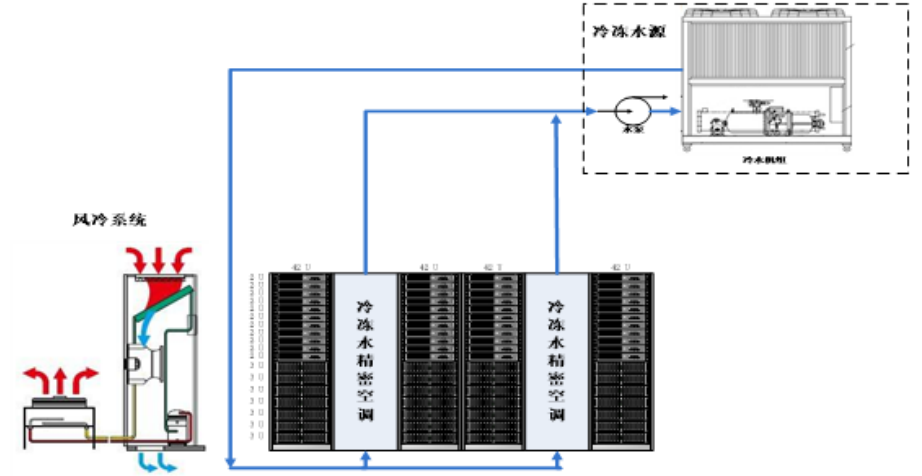
- Demand driven network

- High Performance
- Intelligent
- Flexible
- SDN/NFV
- IoT
- 5G
-



Machine Room

- To be a **GREEN** machine room
- The floor space: 600m² (15 beamlines → 90 beamlines)
 - 100 racks (30 racks for phase I)
 - High-density racks (Comping resources) and General racks (Storage, Network...resources)



- Supporting space: 200m²
 - Power
 - Fire Protection
 - ...
- Power Capacity: 3300kW



计划

- 近期 2019年内
 - 继续深入理解实验及数据处理自动化业务流程: BSRF, SSRF, EXFEL, ESRF, Diamond, PSI , HEPS
 - 加入国际类似装置的联盟, 发起国内光源类设施相关工作的联盟, 开展合作及成果共享
 - 数据管理、数据格式转换、**软件框架**、资源组织方式等设计思路
- 中期 2019-, HEPS光束线建成前
 - 在BSRF上选取若干数线站(如漫散射站、成像站、XAFS、生物大分子站等)对如下工作进行设计、开发、测试
 - 元数据标准制定、抽取、元数据库建设
 - 数据本地存储、数据中心存储、(准)实时数据传输系统搭建
 - 本地数据处理集群建设、云计算处理
 - 软件框架。。。
 - 接口对接、集成等
 - 以上工作如下的调研同步进行(并根据需要进行更新)
 - 线站对数据存储、计算等的要求
 - 线站对软件框架的要求
 - 其它
- 远期
 - 在HEPS线站进行建设、部署, 并根据实际情况进行调整
 - 提供实验数据自动化服务

Reference

- Reference:
 - Eur. XFEL , CSNS , ESRF ,
- Test-bed
 - BSRF
 - SSRF
 - ...
- Cooperation ?
 - HEPS
 - SHINE
 - SSRF
 - CSNS
 - HSRF
 - ...



Big Data Science at SSRF - A Next Generation Superfacility

Prof. Alessandro Sepe
Head of the Big Data Science Center

大科学装置数据科学研讨会
2018.10.21 上海科技大学

Overview of SHINE and Its Data System

Ping HUAI (怀平)
Beamline and Endstations SHINE,
ShanghaiTech University



中国散裂中子源
21 Oct, 2018 Shanghai

Software Architecture of
Data Analysis & Management for CSNS

Junrong ZHANG, Ming TANG, Yakang LI, Fazhi QI
Institute of High Energy Physics

CHINESE ACADEMY OF SCIENCES

Control, data acquisition, management and analysis

Thomas M. Baumann
Scientific Instrument SQS

Hans Fangohr
Control & Analysis Software

SQS Early User Workshop
Schenefeld, 12.02.2018

European XFEL



Data Acquisition and Management Services at European XFEL

Djelloul Boukhelef

for ITDM

Karabo 2.0 workshop

DESY, Hamburg 24.01.2017

European XFEL



总结及讨论

- HEPS是一个用户类设施...软件和服务层面大量工作需要做，希望能借鉴高能所、高能物理领域的成果和合作模式
- 软件框架
 - 在线分析、离线分析、数据管理？甚至包括控制？
 - 是否有可能统一框架？
- 接口
 - 科学数据接口：仅仅同控制系统接口？同控制系统/DAQ分别有接口？
- 合作
 - 用户类设施 + 高能物理实验？共同性、区别？
 - 人员缺口严重
 - 推荐人才：职工、研究生、博士后

谢谢

深化设计报告

- 每一部分可以独立为一个设计报告，能够基于该报告开展合作交流；
其它系统、其它设施、协作研发
- 每一部分需要描述出同外部相关系统和部分的接口
- 整合起来之后是一个完整的HEPS IT深化设计方案
- 图文并茂、既有总体设计、也有细节描述，具有可操作性
- 占到用户视角（线站、科学家、用户）和IT提供者视角描述提供的服务
- 尽早发布、寻求合作
 - 评审
 - 得到认可，讨论、合作
 - 合作的原则：共性合作、不共性的共享思路，

深化设计报告

- 总体设计报告(Overview)
 - 目标、理念、设计思路、包括的内容
 - 实施计划
- 基础设施
 - 机房
 - 网络：总体设计思路和架构，描述出几张不同的网络之间的关系、关键技术指标、互相之间的接口、各自的功能和承载业务，涉及到的关键技术（甚至包括需要预研验证的）；面向别的系统
 - 存储：总体设计思路和架构，根据业务需求介绍资源组织方式（逻辑集中，物理上可以集中，也可以分离，根据具体使用场景，如线站缓存？数据中心集中存储？长期保存？）和服务场景、性能指标；分别占到用户的角度和IT设施提供者的角度描述资源服务流程；涉及到的关键技术，涉及到的关键技术（甚至包括需要预研验证的）
 - 计算：总体设计思路和架构，根据业务需求介绍资源组织方式（逻辑集中，物理上可以集中，也可以分离，根据具体使用场景）和服务场景、性能指标；分别占到用户的角度和IT设施提供者的角度描述资源服务流程；涉及到的关键技术（甚至包括需要预研验证的）
 - 设施统一安装与管理：总体方案、实现技术、服务场景、关键指标
 - 安全：
- 科学数据获取：
- 科学数据管理
 - 总体描述科研数据生命周期，每一个过程中数据管理的功能、输入、输出、接口
 - 科学数据服务portal及其后端关联系统及技术
 - 软件实现的思路及每一部分的具体实现方案
- 科学数据获取与分析（软件框架及软件集成）
 - 总体描述需求，围绕数据生命周期，数据分析的分类和特点，和数据管理的关系，和其它系统的关系
 - 在线快速分析、离线分析，软件的功能，对计算和存储资源的特性的需求
 - 软件框架与科学软件之间的关系和业务逻辑，不同视角的描述
 - 软件实现的思路及每一部分的实现方案
- 设施运行支撑软件
 - 总体描述需求，围绕实验生命周期，包含的支撑软件
 - 用户管理、权限管理、提案管理、实验过程管理、.....
 - 设施资产管理、设施运行数据管理与分析、...
 - 软件实现的思路及每一部分实现方案

深化设计报告

- 公共支撑平台
 - 关系型数据库
 - 非关系型数据库
 - 公共软件库管理及服务平台
 - 代码管理平台
 - 智能化运行监控中心（包括运行和安全）
- 预研、测试及合作计划
 - 每一个工作均要涉及
 - 预研目标、指标、计划的线站
 - 合作的单位、要求