MOCPL02, Monday Oct 7th, ICALECPS 2019, **Brooklyn, New York City**

HZB Helmholtz Zentrum Berlin

Modernization of Experimental Data Taking at BESSY II

Roland Müller, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH *roland.mueller@helmholtz-berlin.de*

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Modernization: Why, How, Where to

Motivation: Problem Description

- Specific User Service @ BESSY
- Decentral Organisation @ HZB
- Reorganisation Needs

Analysis: Options and Strategies

- Facility wide Integration Standard to be agreed on: EPICS
- Flow control: Community co-developed Software Stacks
- Beamline Digital Twin: Modelling, Machine Learning

Future: Novel Instruments, Perspectives, Outlook

- Adopt to emerging Needs and Capabilities
- Data driven Science (4th Paradigm)

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Background: BESSY – Beamline Controls Environment

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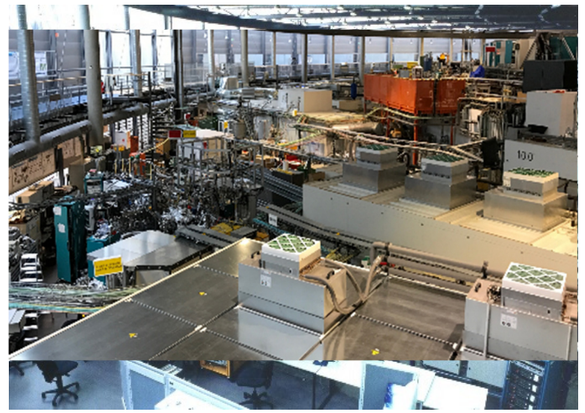
“20 years ago” – BESSY II initial user service mission:

- Only Open Port + cooperating research group (CRG) beamlines (BL)
- Rapid Ramp Up to ~35 BL, 50 Instruments
- „Standardized“ hardware, „Centralized“ BL support



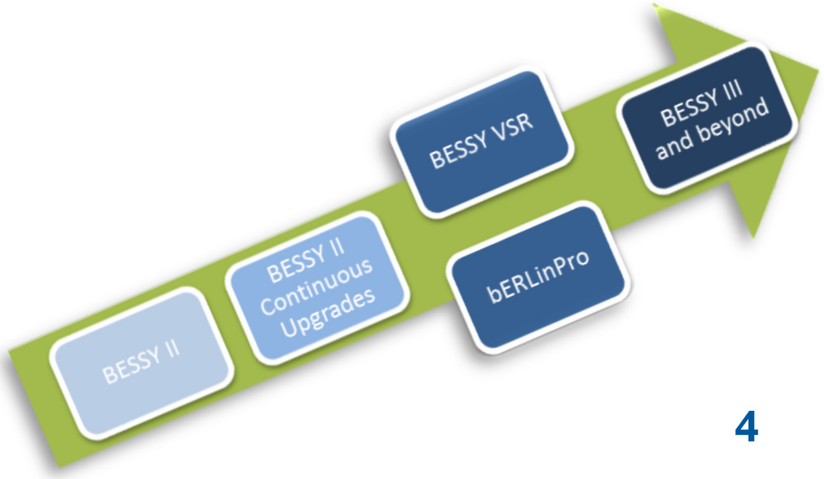
“10 years ago” – 2009 BESSY II / HMI fusion into HZB:

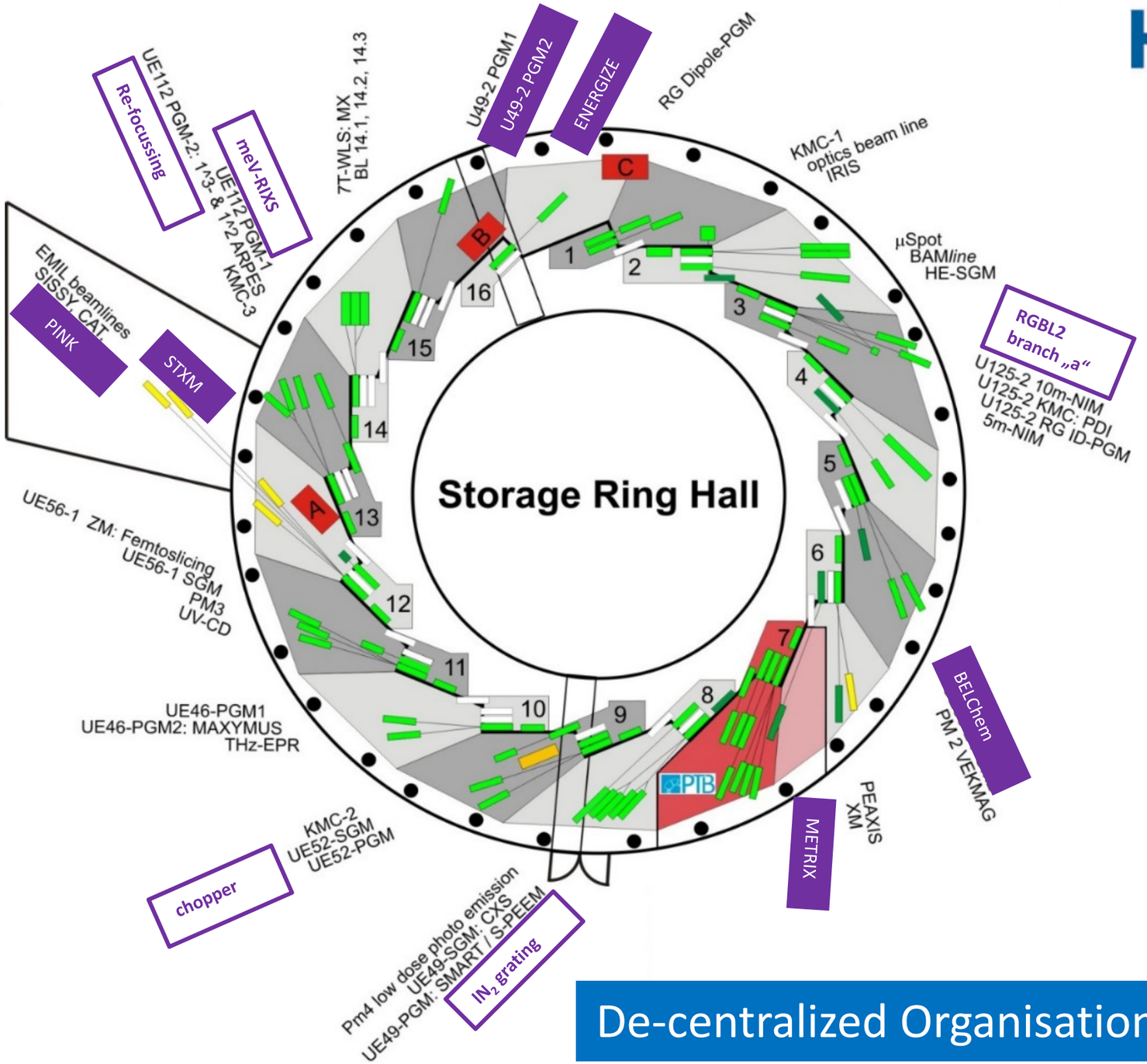
- Two facilities: light source (X-rays), nuclear reactor (neutrons)
- One, material science focused, user platform
- New developments along Projects setting up instruments
- Technical Support staff Decentralized into scientific units

10 20 JAHRE VOLLER ENERGIE VOLLER LICHTBLICKE

“Today” - Strategic guidelines:

- Shutdown of the reactor at the end of 2019
- New Scientific focus: Renewable energy, materials and technology
- Successor Facility **BESSY III**: “within 10 years from now”





De-centralized Organisation @ BESSY

12 HZB Organizational Entities are responsible for instruments

ASD
AME
IF
IS
ISPEK
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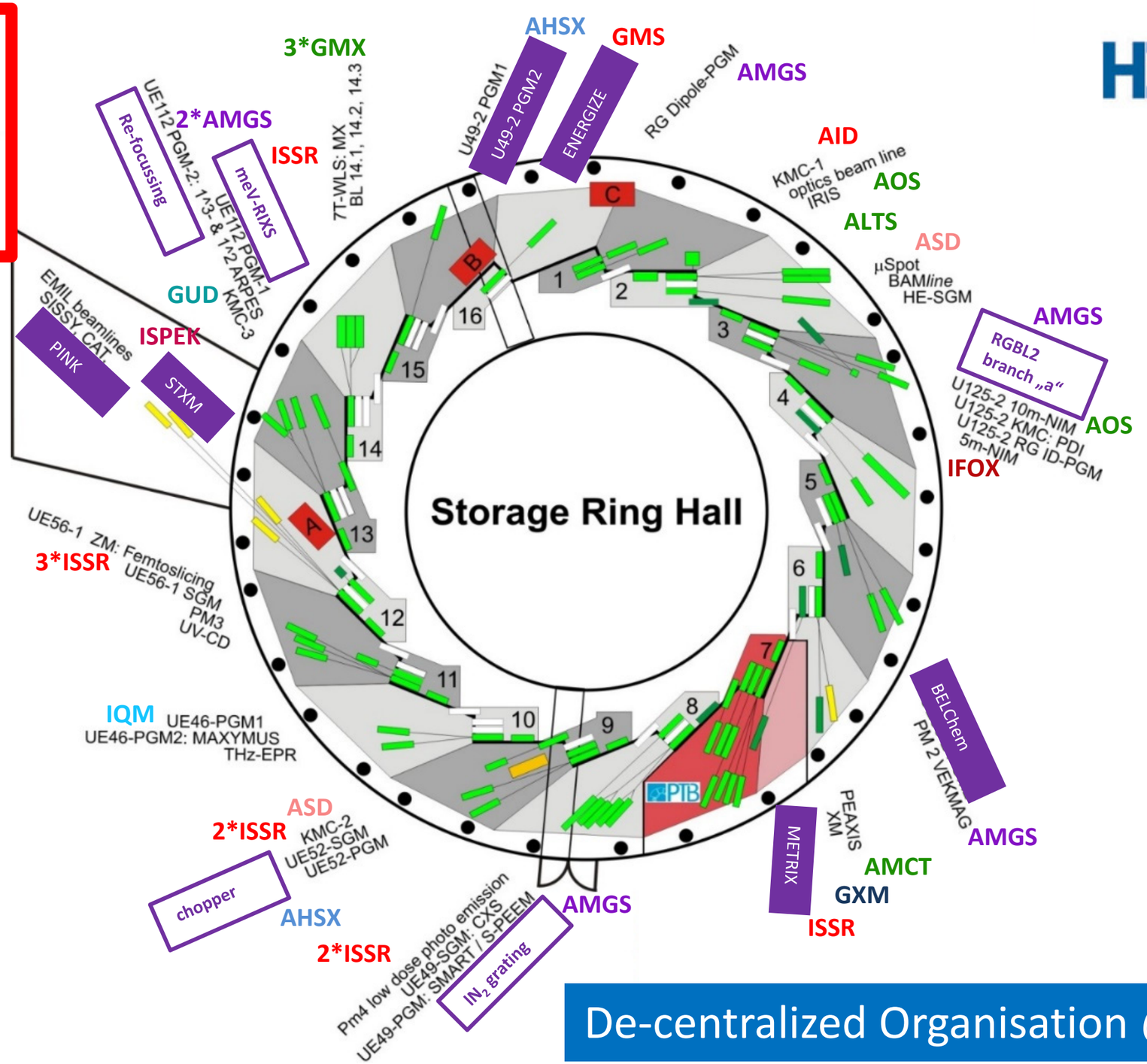
PvComB



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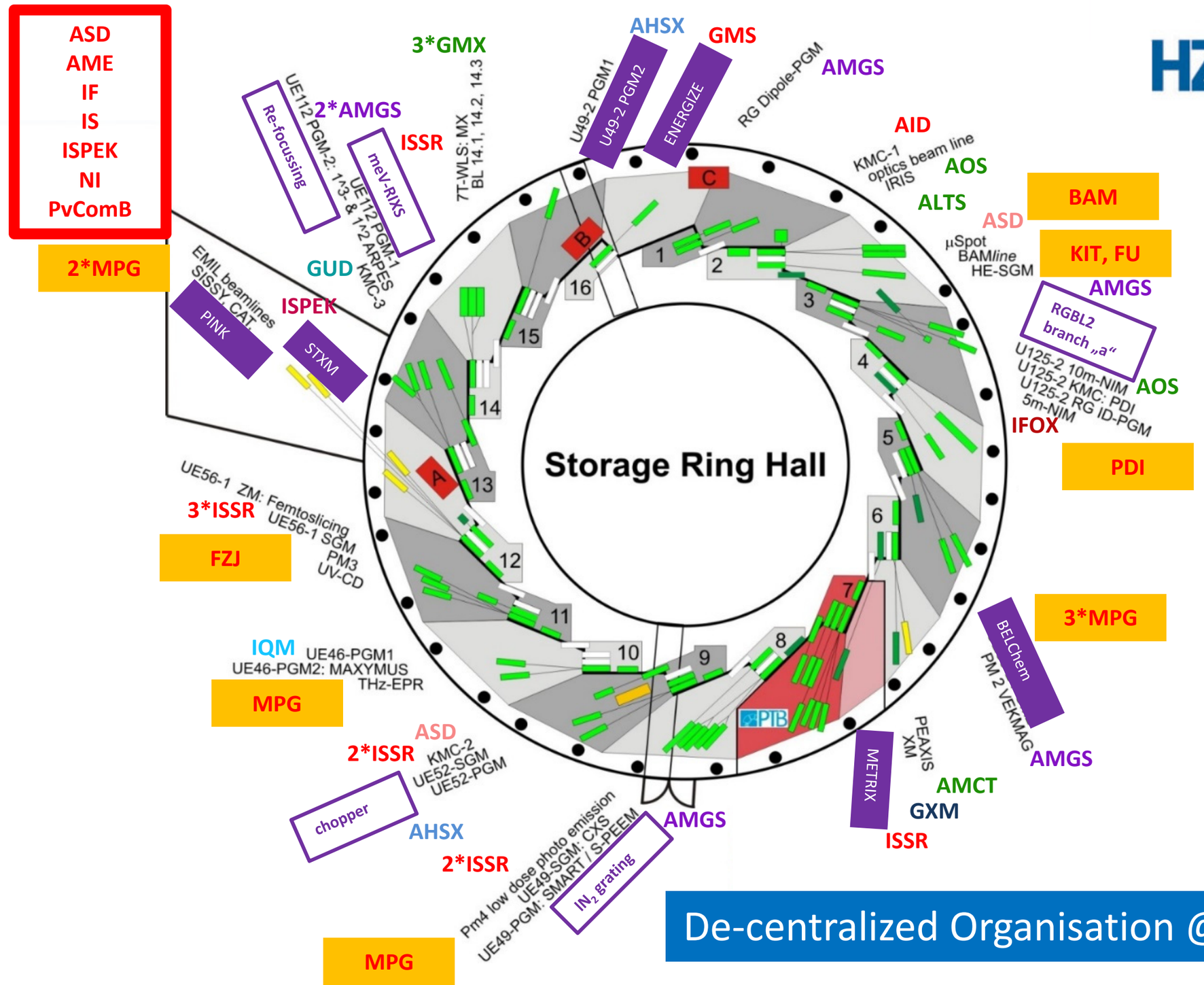

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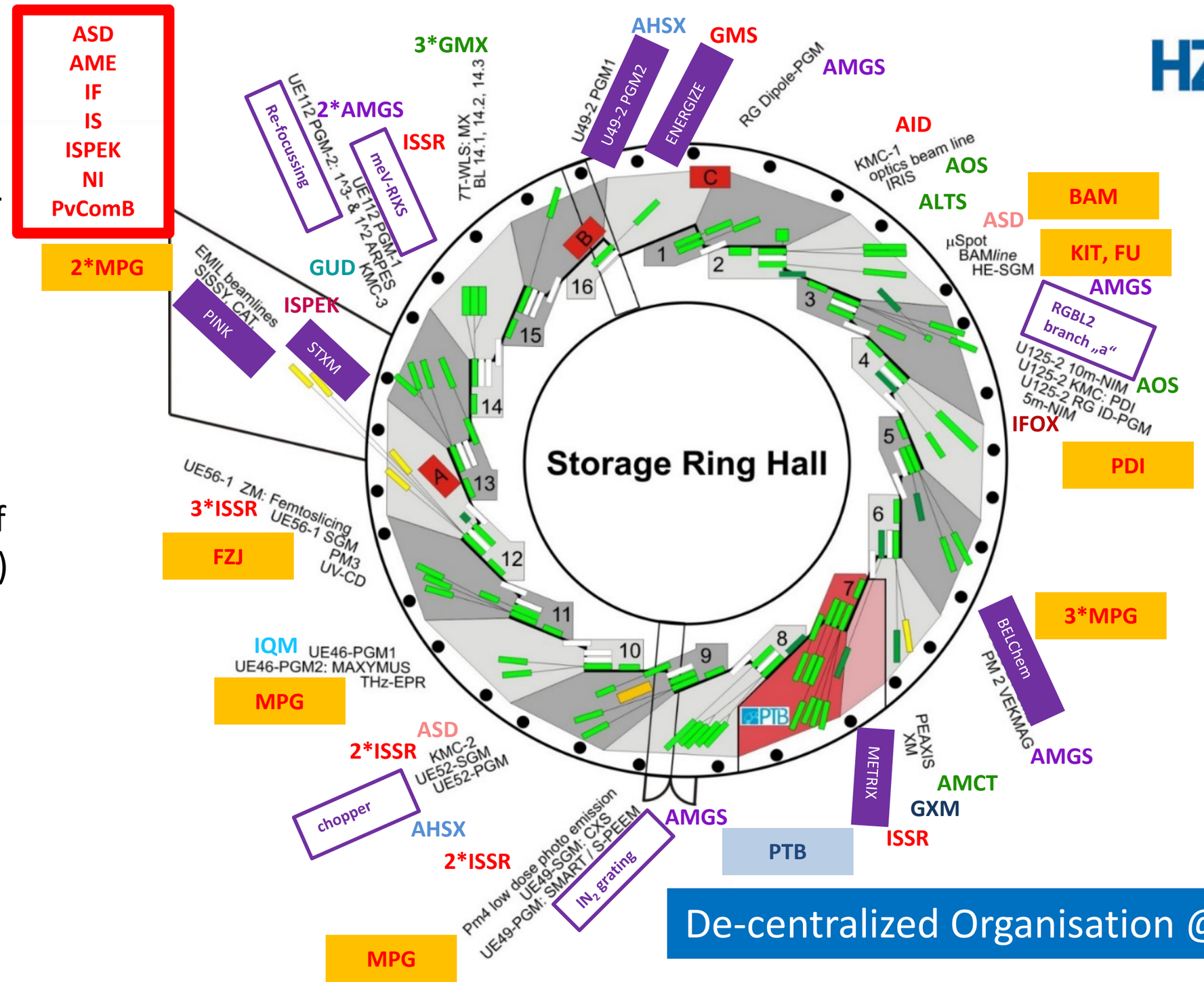
1 separate Lab (nat. Bureau of Standards,PTB)



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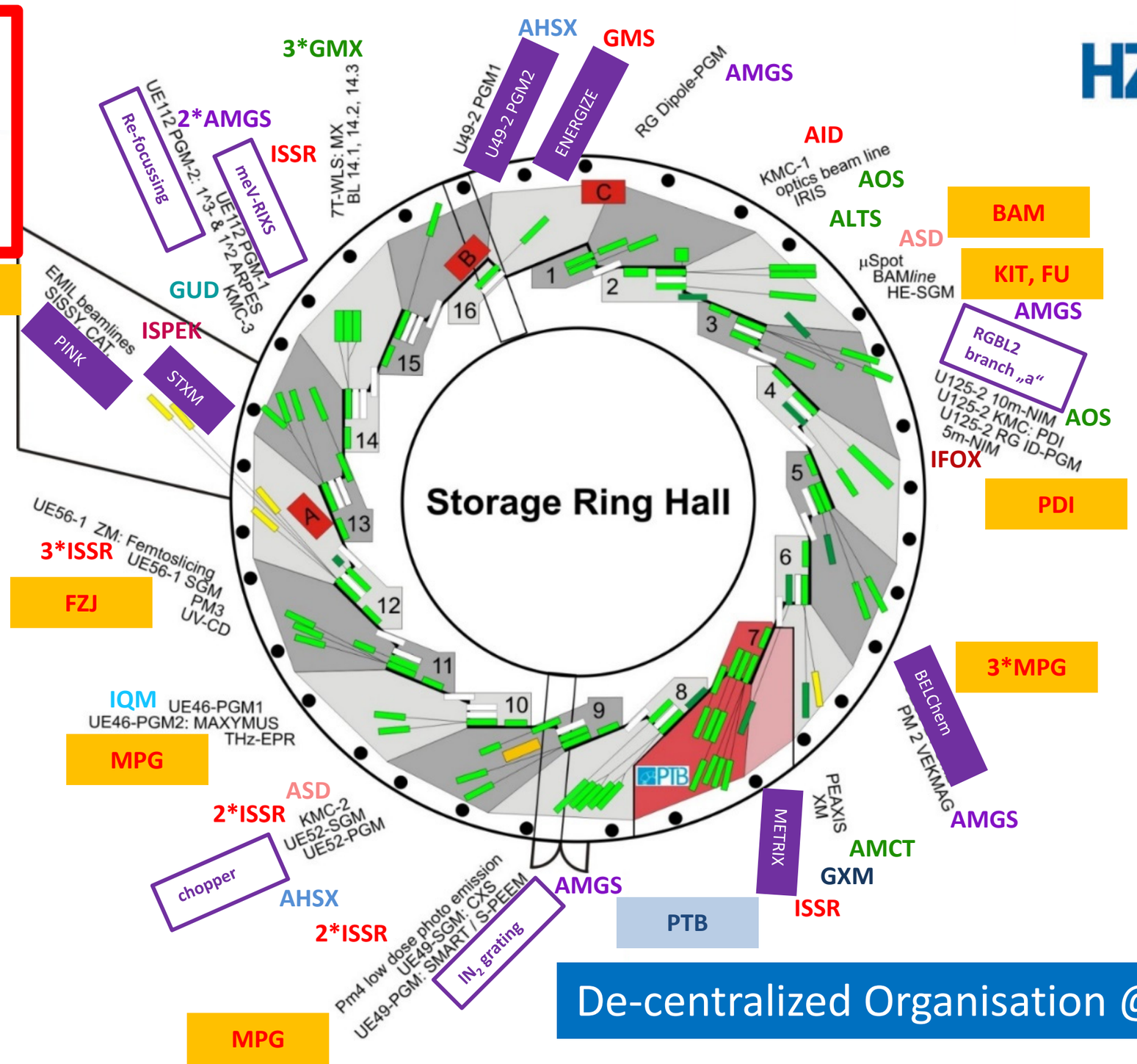
Beamline, ID Control most use generic control program: **MONO**



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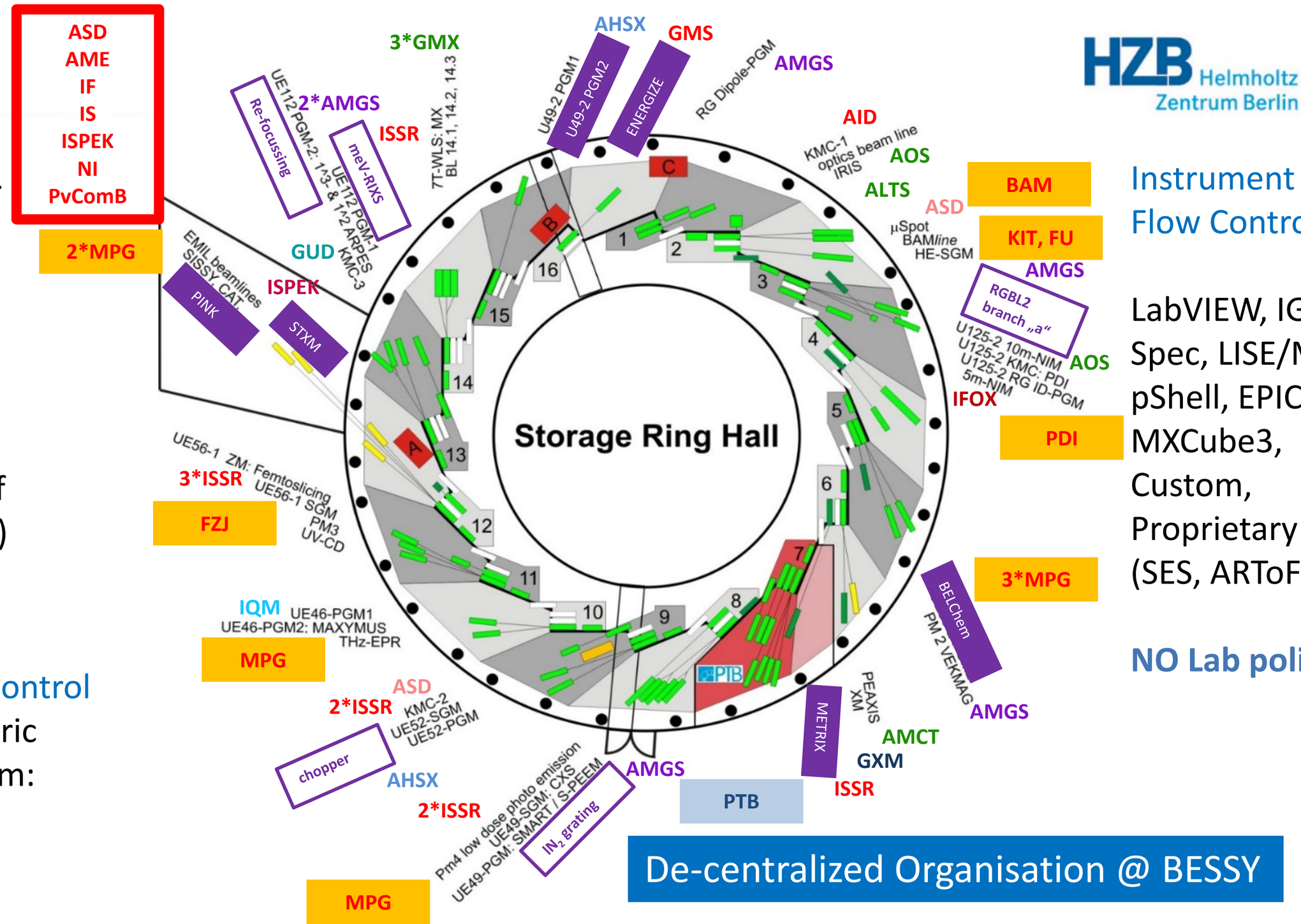


Instrument + Flow Controls

LabVIEW, IGOR, Spec, LISE/M, pShell, EPICS, MXCube3, Custom, Proprietary (SES, ARToF)...

NO Lab policy

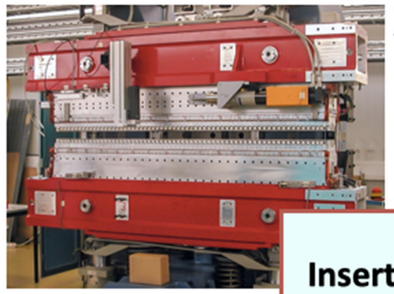
De-centralized Organisation @ BESSY

Beamline Control: Central Component, once Enabling

Monolithic, multipurpose, generic software **MONO**

- Enabled fast roll-out of now ~50 beamlines
- Integrates new BL components, Insertion devices
- Central to legacy experimental control infrastructure
- Hard to maintain, develop, extend

High level applications: close to anarchy



X-ray Source

X-ray Source: Beamline/ID Simulation Software

Digital User Office

Insertion Device(ID) hardware

Beamline

Beamline hardware
Motor
Encoder

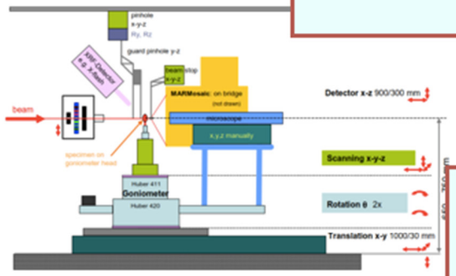
Fly Mode Synchron

MONO

Graphical user interface

Experiment flow control

Experiment Hardware, Detector



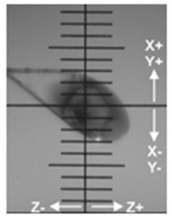
DAQ, Area Detector

Live evaluation during the measurement

User

Data Storage

Sample Environment



Instrument

Software

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Integration Ordering Principle: EPICS

Low Level: EPICS PV connectivity

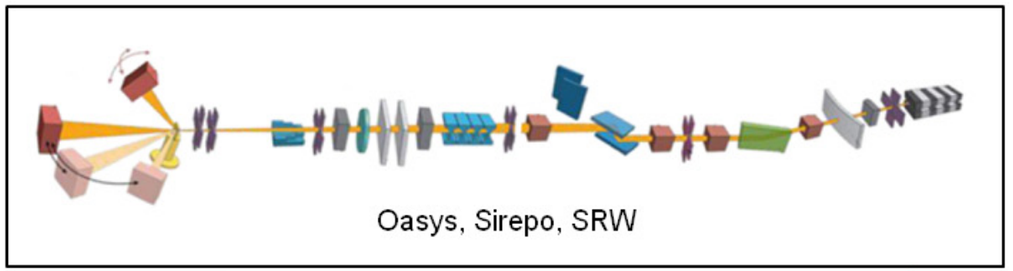
- LabVIEW based solutions
- Proprietary detector access
- Slow controls of fast DAQ
- PLC based subsystems
- Complex components
- Alien controls units

High Level Controls: HW abstraction

- Prime candidate for Device Data Model: ophyd

Meta-goal: provide a common dataset (accelerator, beamline, instrument) describing experimental conditions.

For data driven science purposes the experimental floor is in the dark today.



Software Stack
pShell, Bluesky, pyDM

Workflow
DAQUIRE, Kepler

EPICS tools
CSS, Archiver, Alarms

Evaluate
FOSS,DPDAK, IGOR

Exp. App.
Scan, grab

Modelling
Digital twin

EPICS Channel Access

Simple Devices
Keithley, Thermocouple

PLC
Safety, Interlocks

Slow DAQ
Fast Detectors

spec
Legacy Systems

LabView
Special Equipment

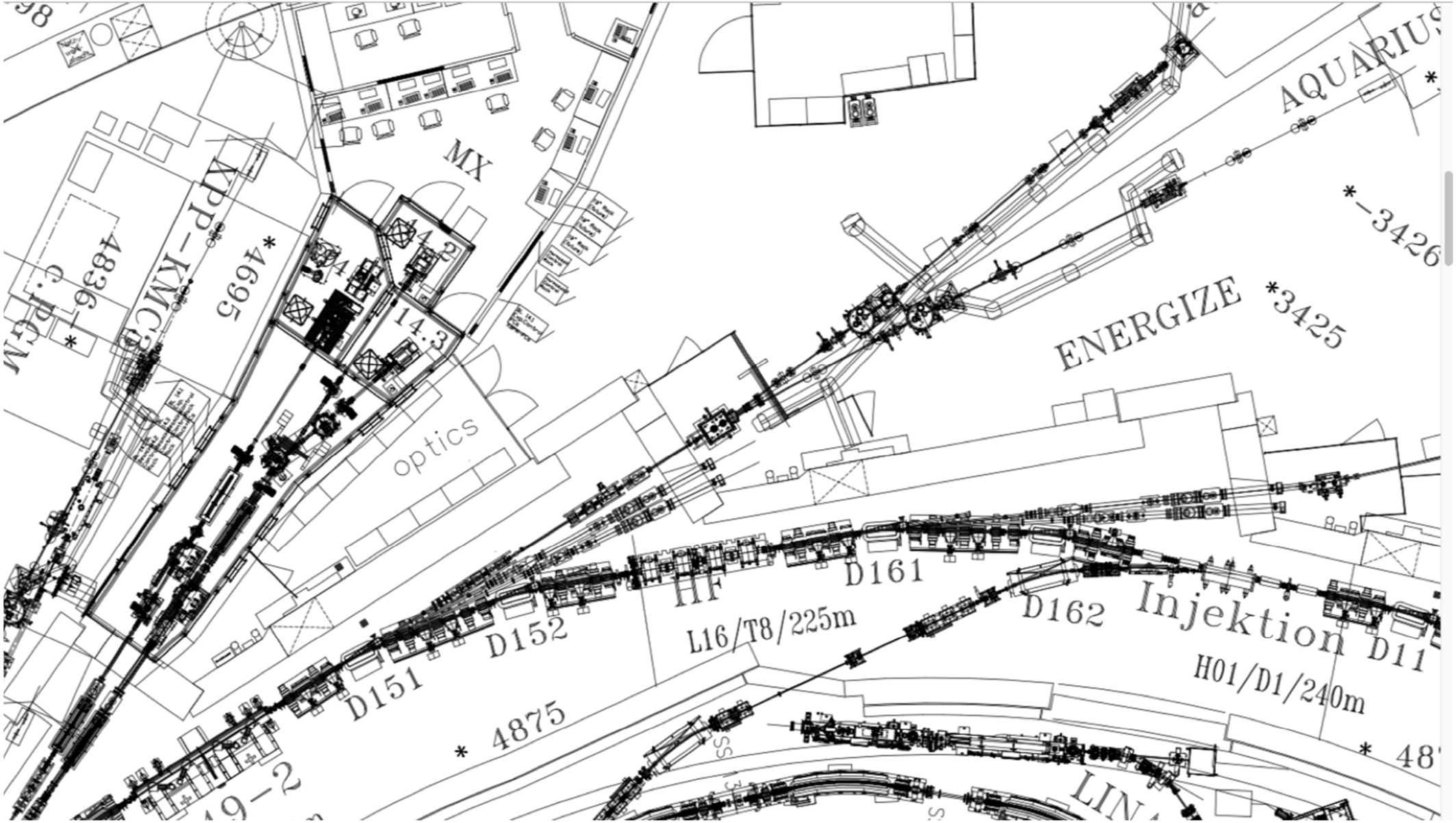
LISE/TANGO
Complex Instrument

SeCop
Sample Environment

Begins with Naming Convention: Nontrivial for Shared Devices

Challenges for conflict-free naming:
ID-BLs split into several (up to 2*3) branches with no clear geometric order/hierarchy

The individual instrument changes the hardware representation, functionality and set-point of the common section when active

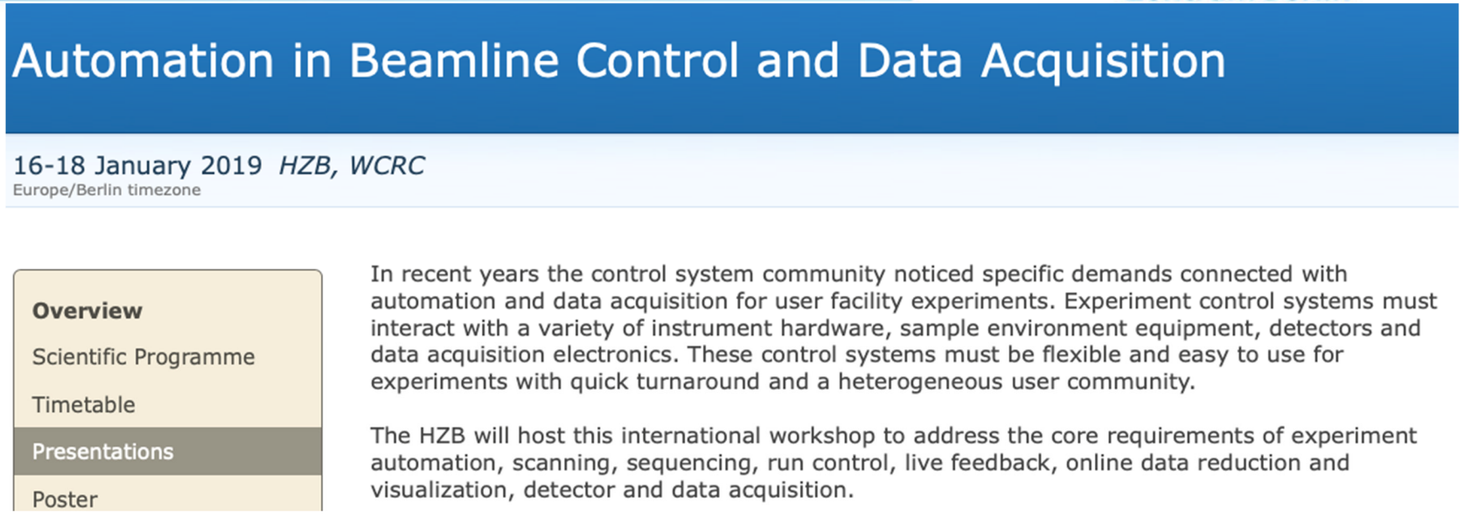


Flow Control Tools

HZB hosted a workshop *Automation in Beamline Control and Data Acquisition*

https://indico.helmholtz-berlin.de/conferenceDisplay.py?confId=11

- community supported tools
- proven outreach and portability
- new trends / requirements in DAQ



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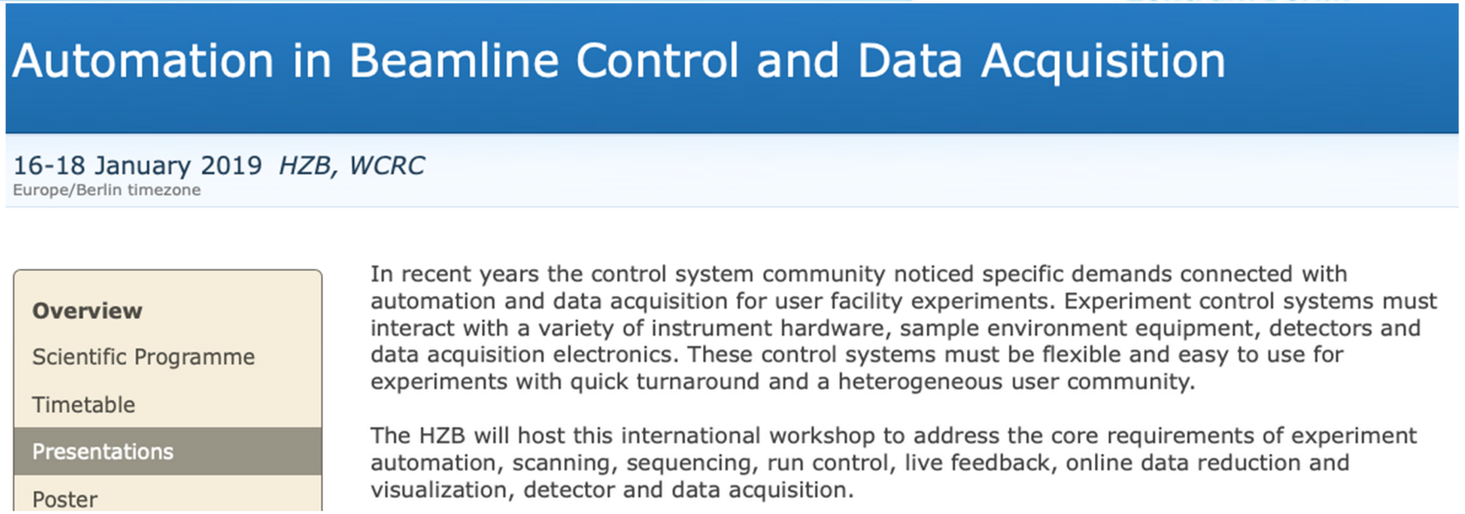
HZB: for flow control the python stack

- Ophyd: device abstraction
- Typhon: GUI generation
- Bluesky: data collection
- pyDM: display manager
- transitions: finite state machines

serves as the role model/benchmark



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serves as the role model/benchmark

For a more complete picture see the proceedings

Bluesky, Ophyd, Transitions: Adequate for Most Complex BLs

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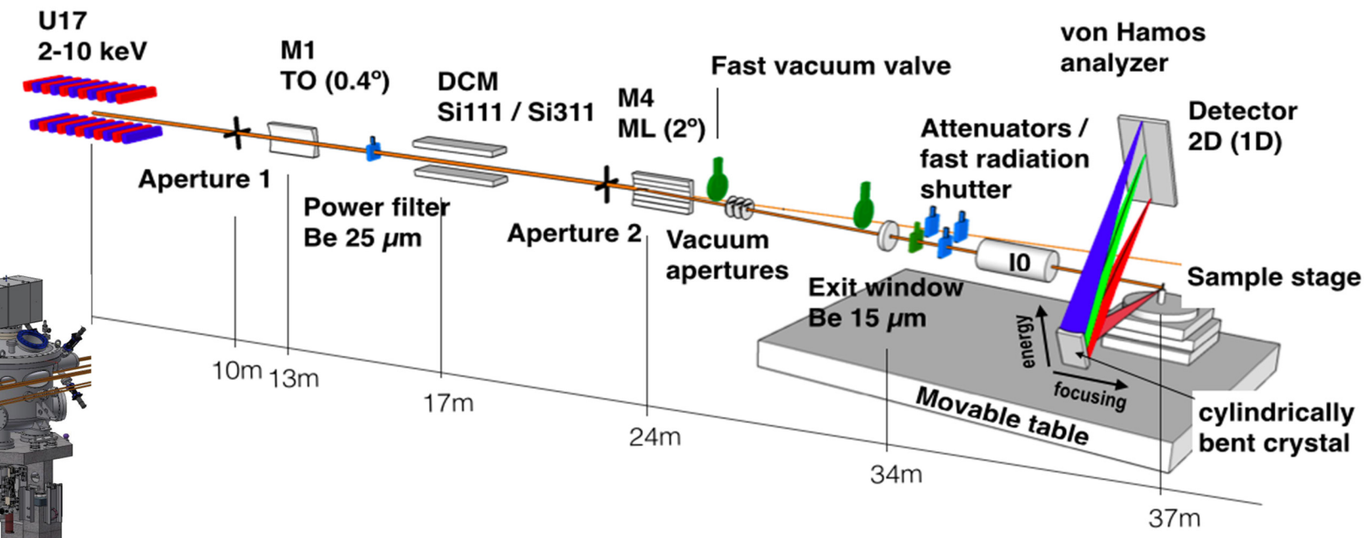
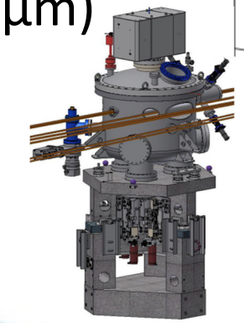
Cutting edge “EMIL”: Active focus control

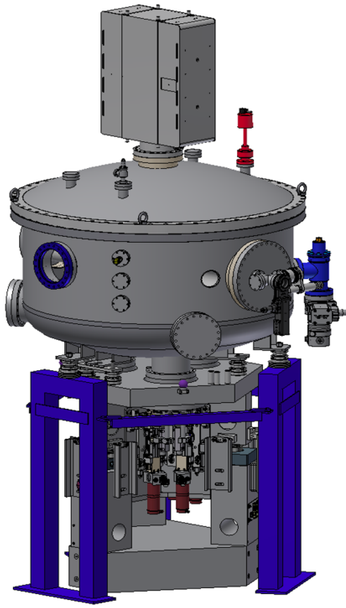
- Intense, sequential usage of beam
- 4 min change time, no thermal equilibrium
- Long beamlines (64m), Small foci (20µm)





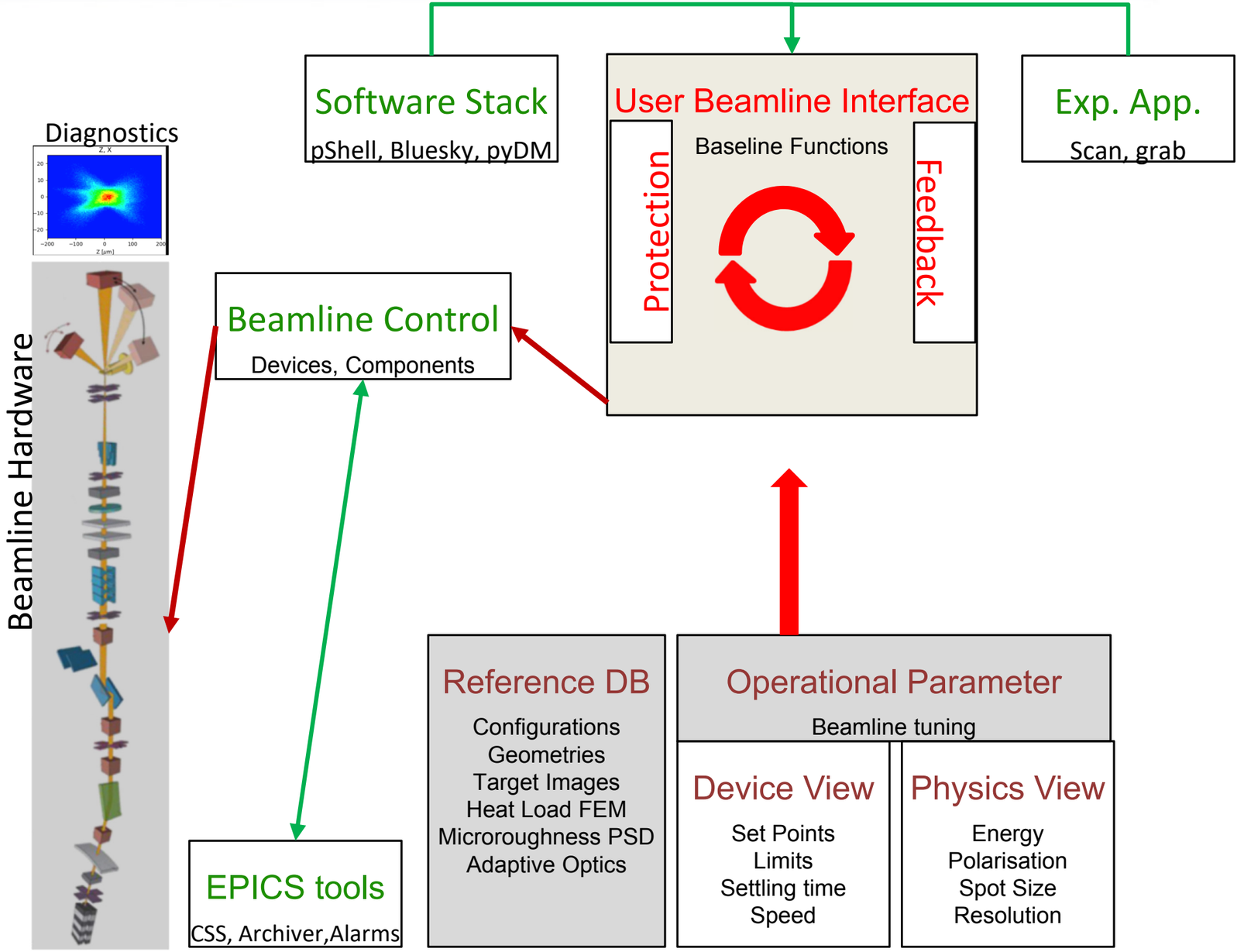
Rapid, precise, coordinated switching:

- Powerful sample robotics @ SISSY I + II
- Hard + soft X-rays on the same sample spot
- 5 competing end stations, 2 source points
- Variable wave length + pol. scan times



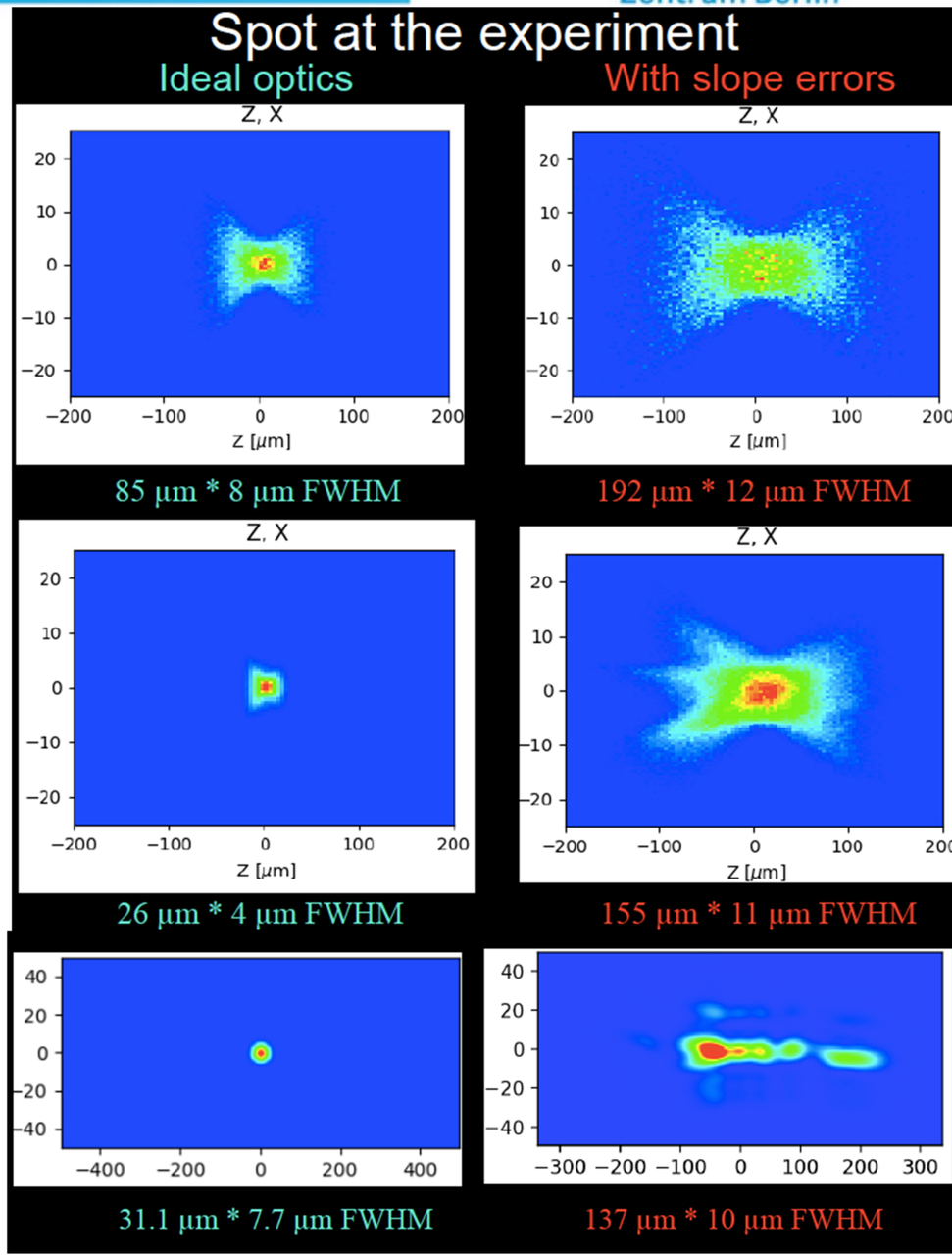
BL Operation Toolset: Plan for MONO Successor

- Accept configurations from reference and operational DB
- Comply to EPICS tools
- Transfer experimental flow control commands to beamline



Role of Realistic Beamline Modelling

- Precise beamline models allow to understand discrepancies between intended source point modifications and observations



RAIMONDI, Lorenzo, Optical systems: from metrology characterization to WFS analysis, through OASYS , Beamline Simulation and Tuning

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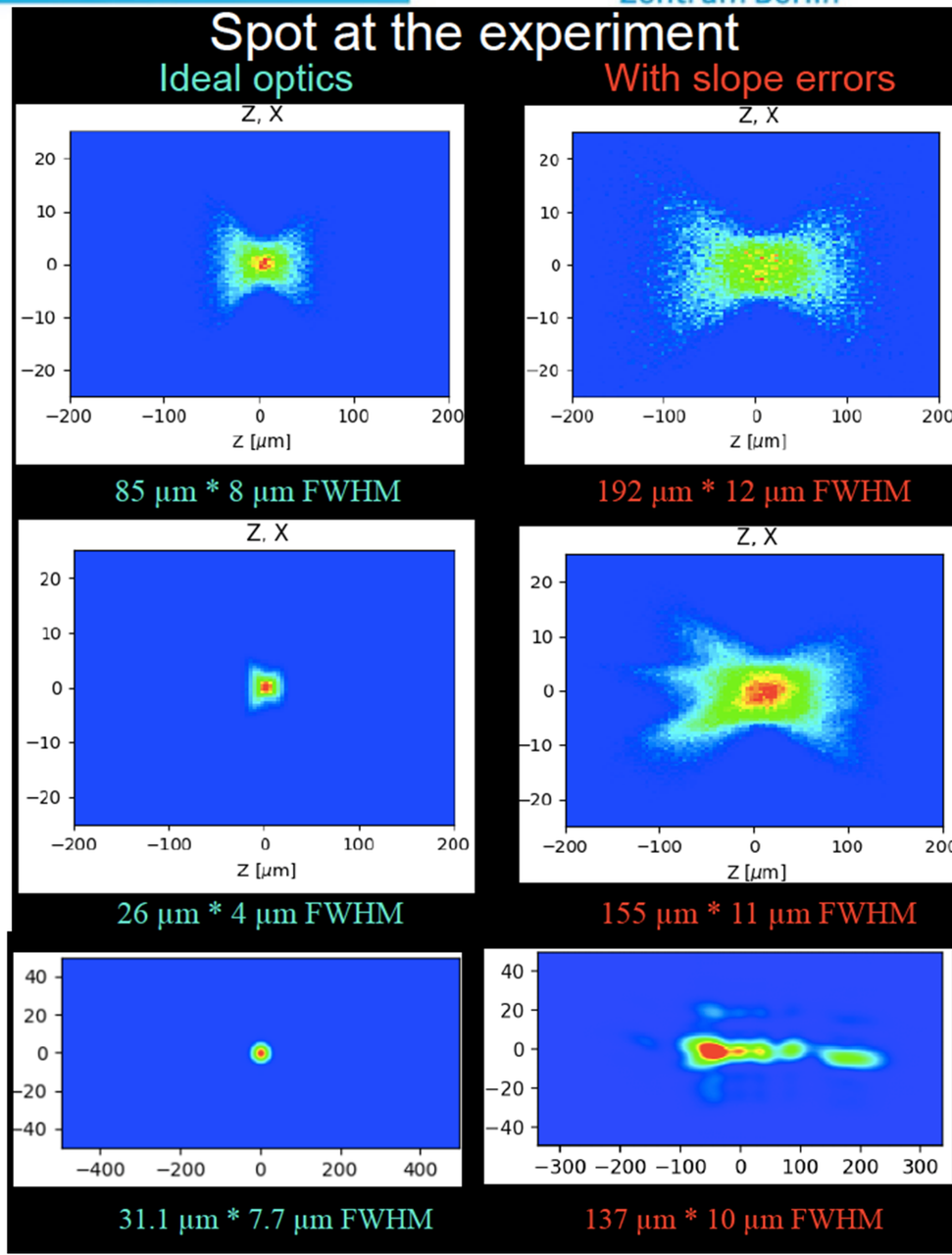
- Goal: capabilities to run simulation of x-ray generation and preparation parallel to the operation of the real installation (*digital twin*).



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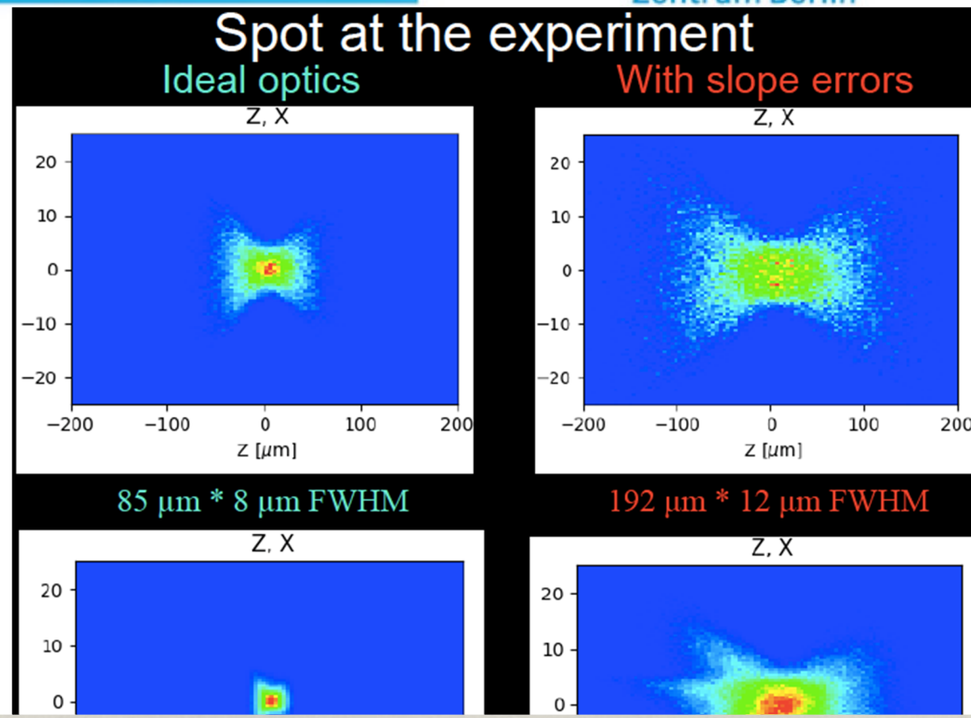
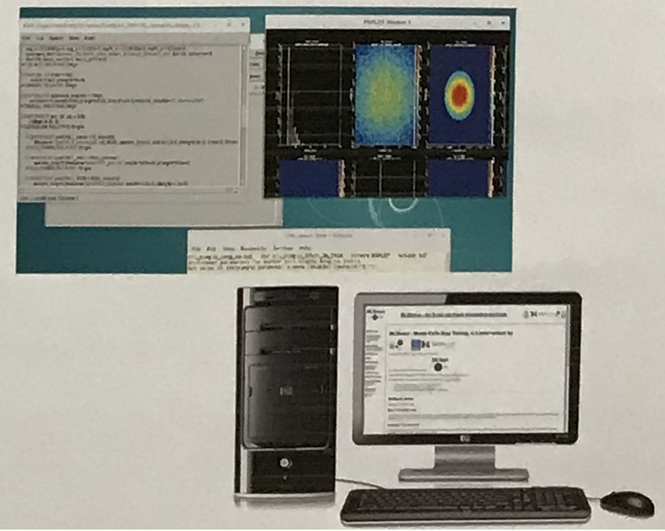
- Role model @ DanMAX beamline MAX IV



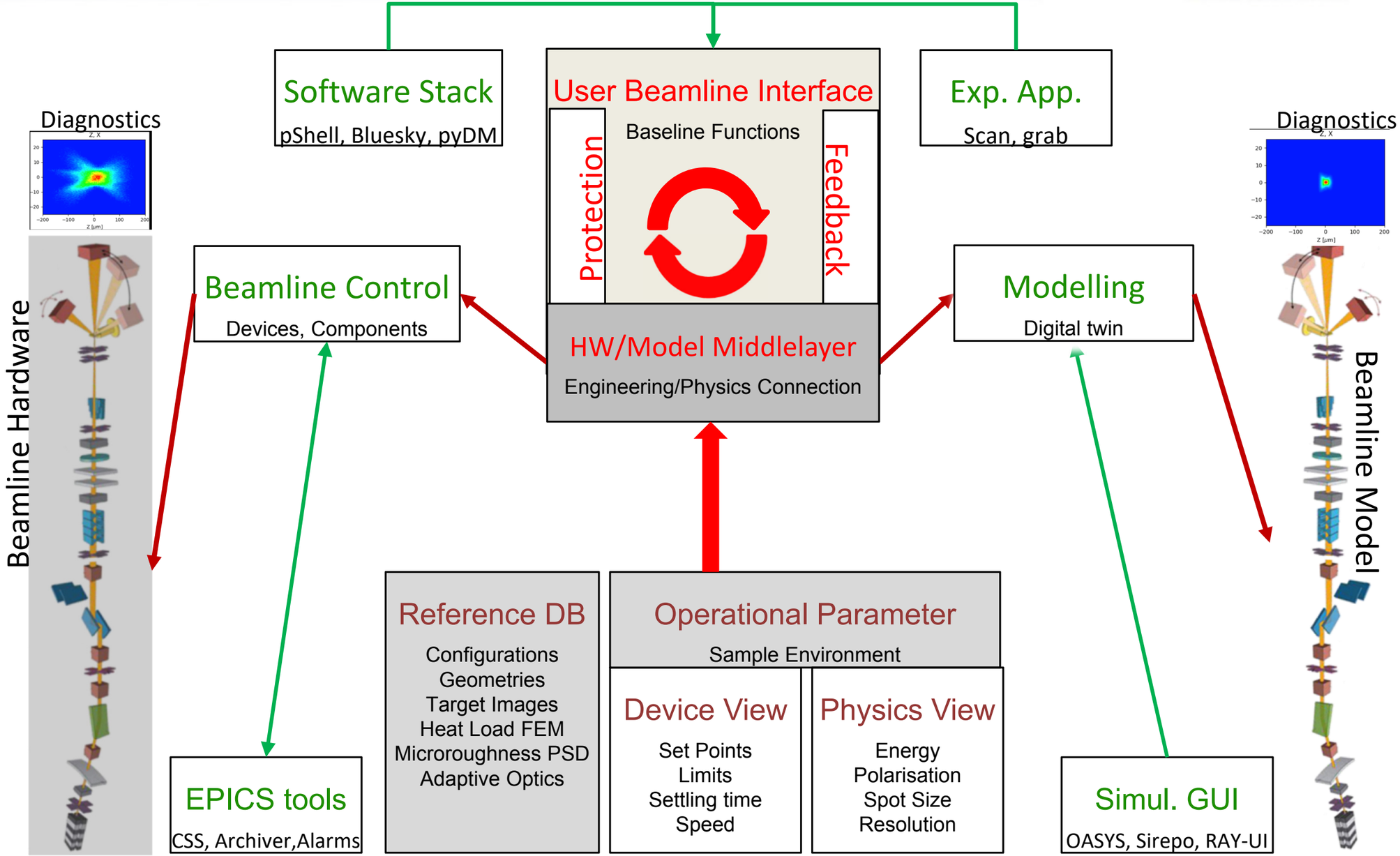
Virtual experiments

Besides the physical beamline a complete virtual model is build in the X-ray ray tracing software McXtrace [mcxtrace.org]. This model will be available on a web server for users to run and test their proposed experiments online before coming to DanMAX to perform the real experiment.



Common OPI to Beamline Operation and Modelling

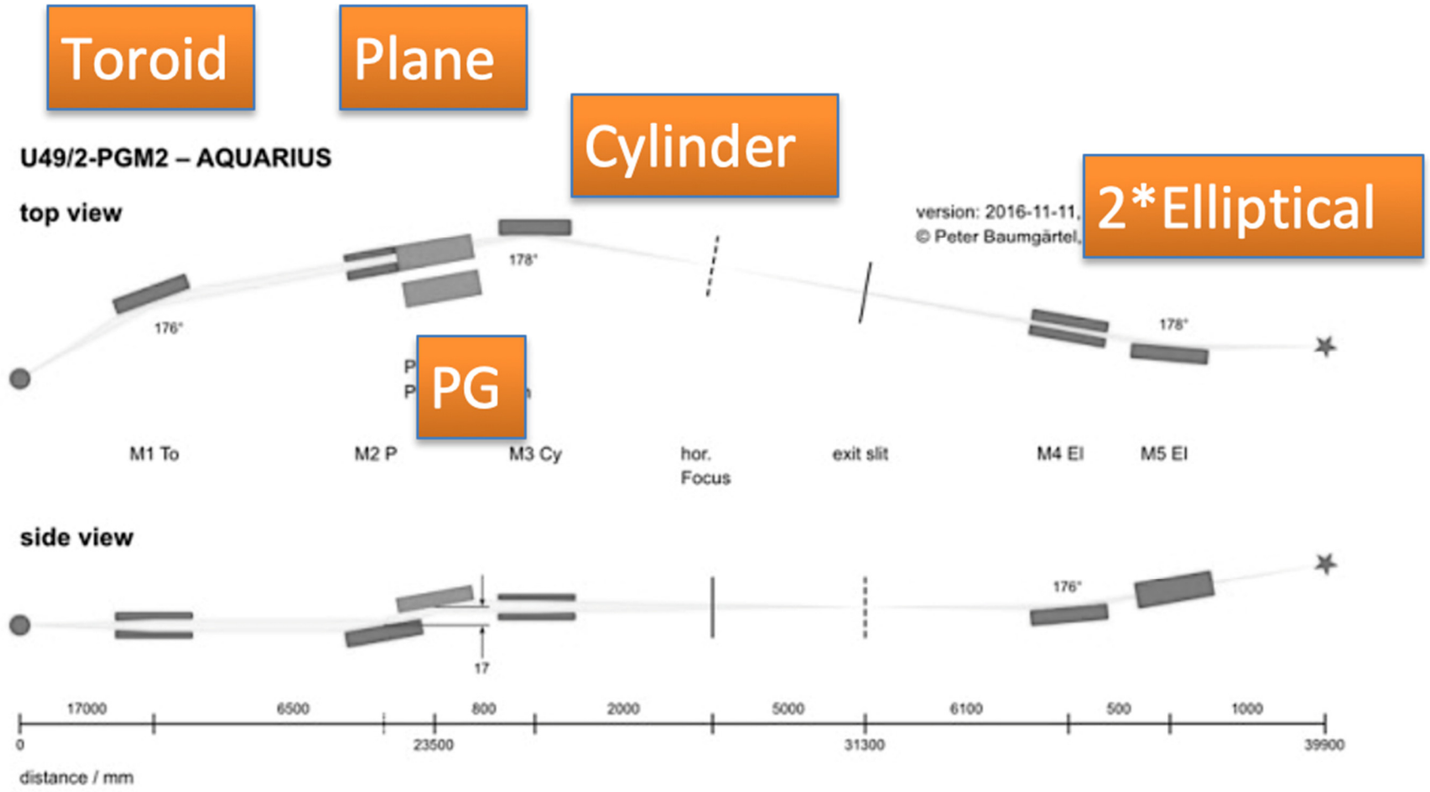
- Middlelayer connecting operation to simulation mode
- Relevant parts of modelling software in server mode
- Method well known at accelerator control



Additional Tool: Machine Learning, Training Data via Simulations

- Proof of principle @ standard beamline

TUCPL01, Luis Vera Ramirez et al., Adding Machine Learning to the Analysis and Optimization Toolsets...



Additional Tool: Machine Learning, Training Data via Simulations

- Analyse x-ray properties at selected positions

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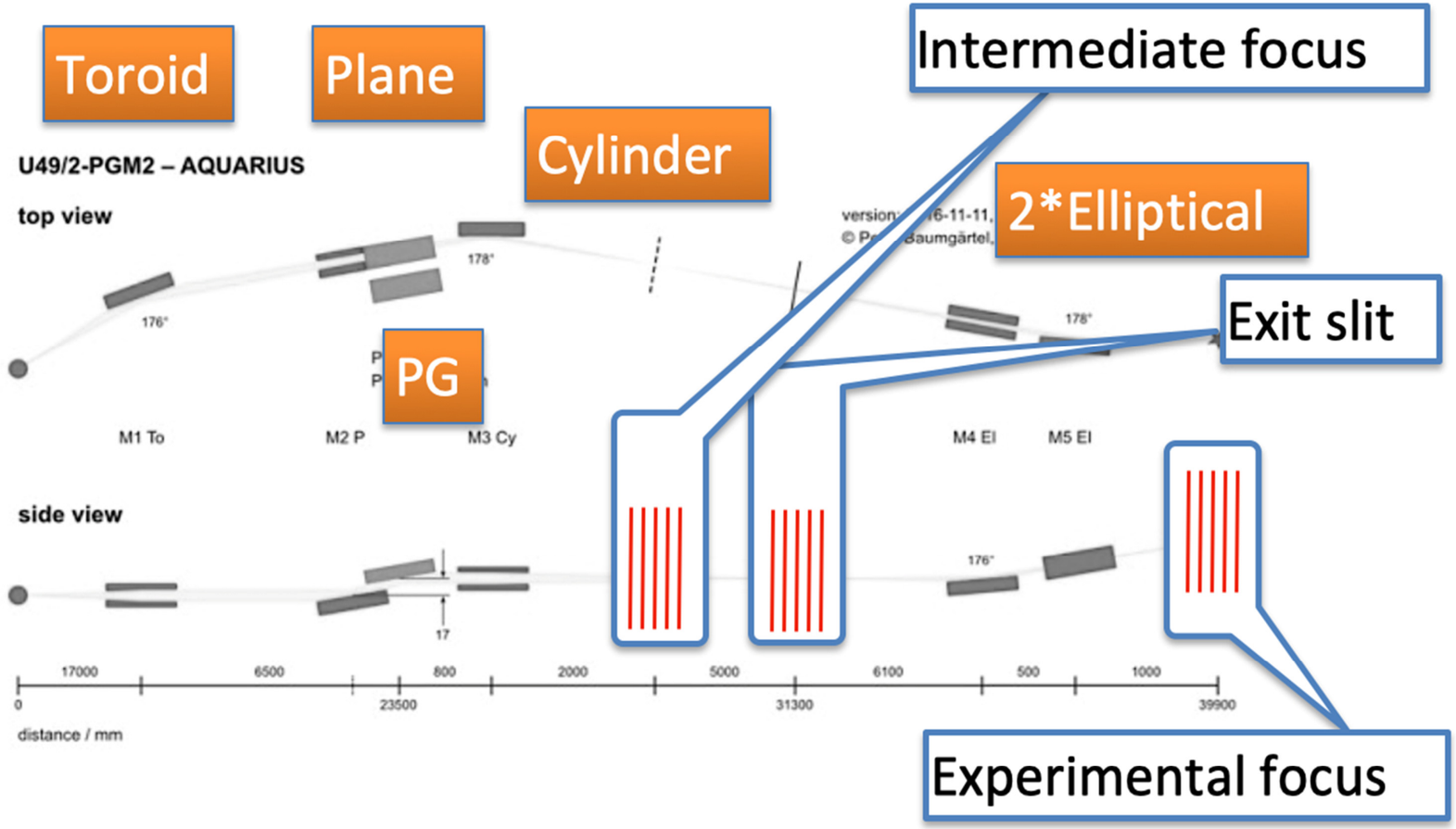

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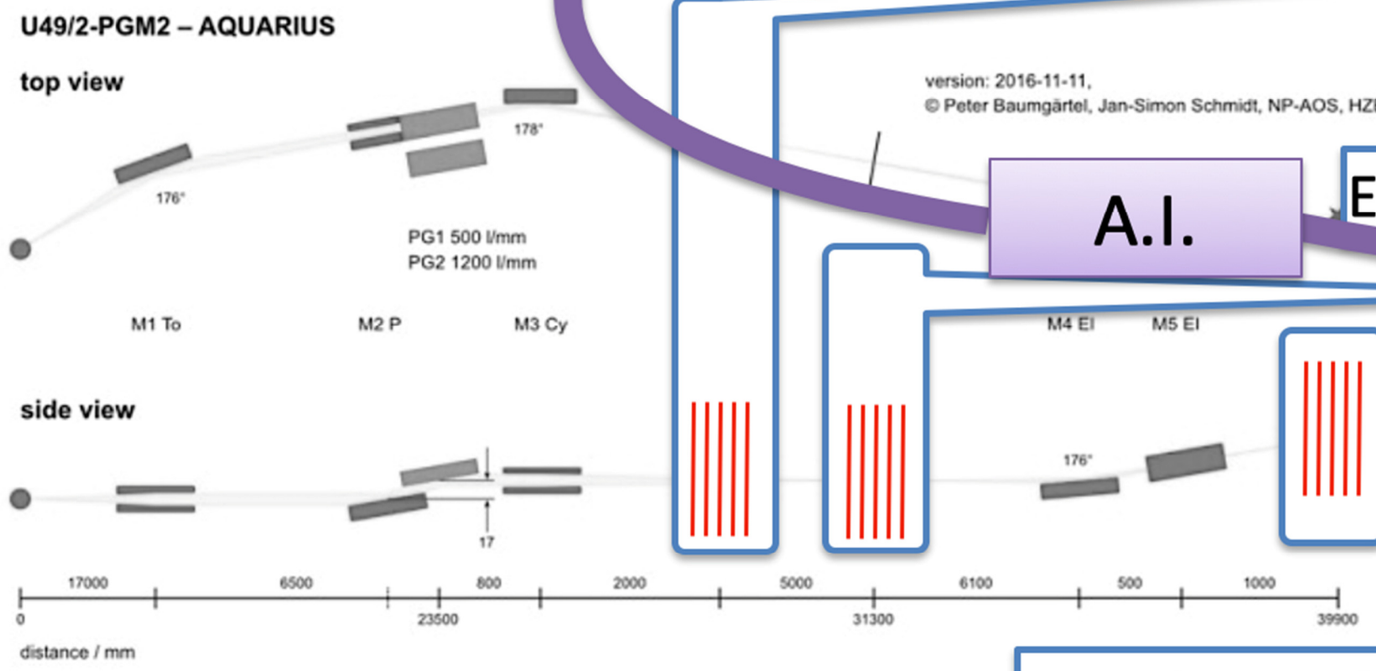
- Hor./ver./long. misalignment/misorientation/offset
- Slope errors
- Long radius
- Entrance arm length
- Line density
- Fix focus constant
- Thermal distortion
- …

~100 parameters varied

One simulation: ~1s
—> rough map: 10^{100}s
—> good map: 100^{100}s

Intermediate focus

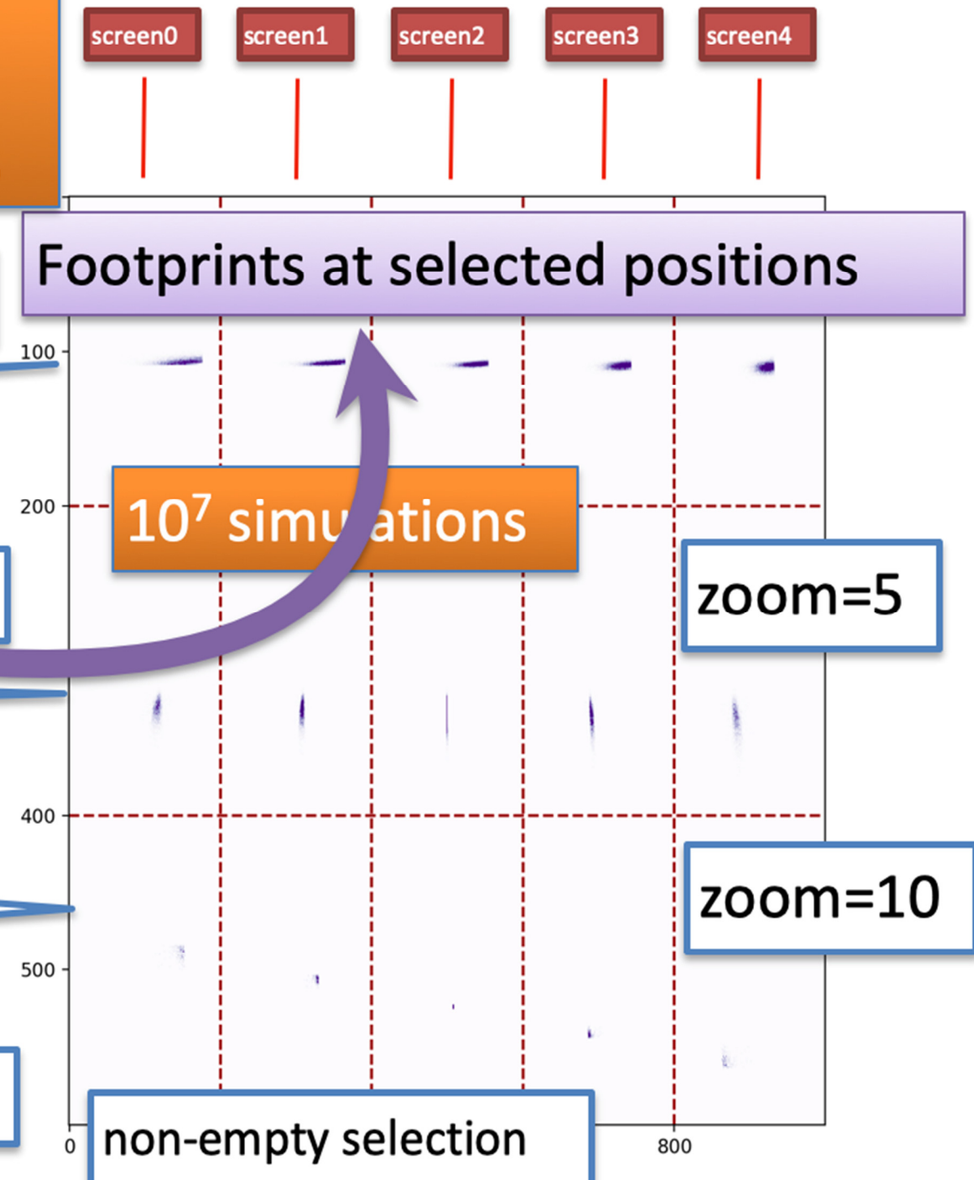


A.I.

Exit slit

Experimental focus

Footprints at selected positions



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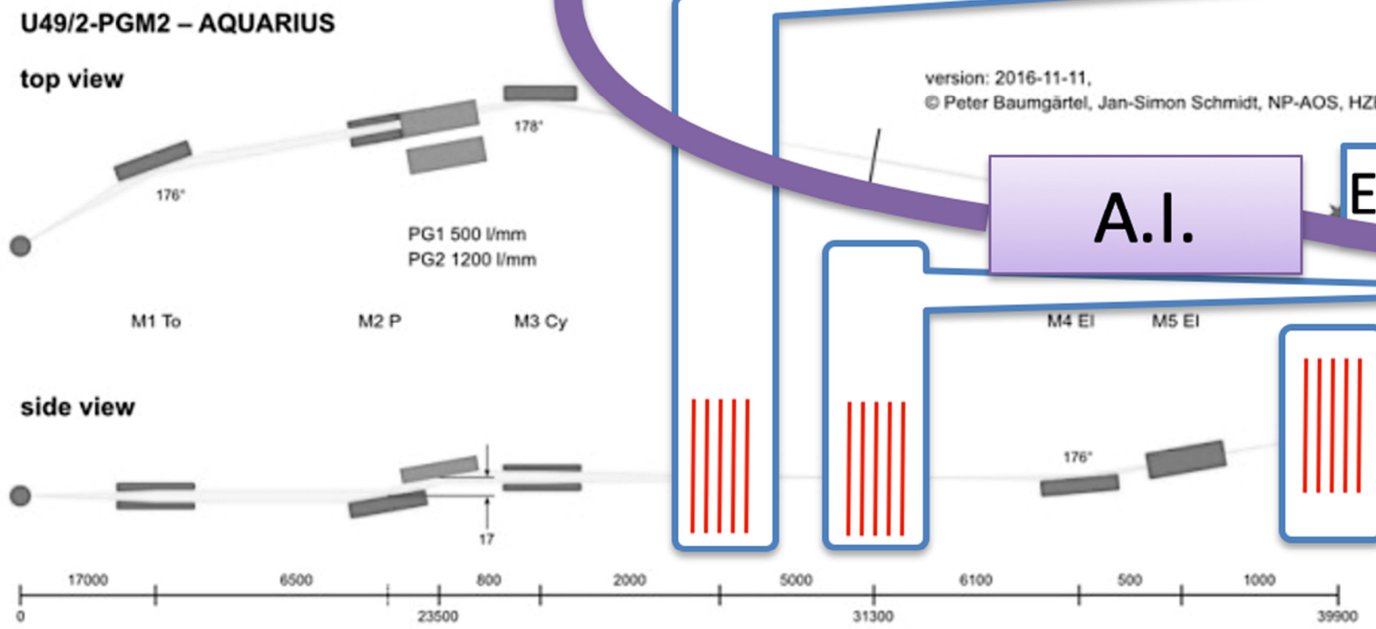

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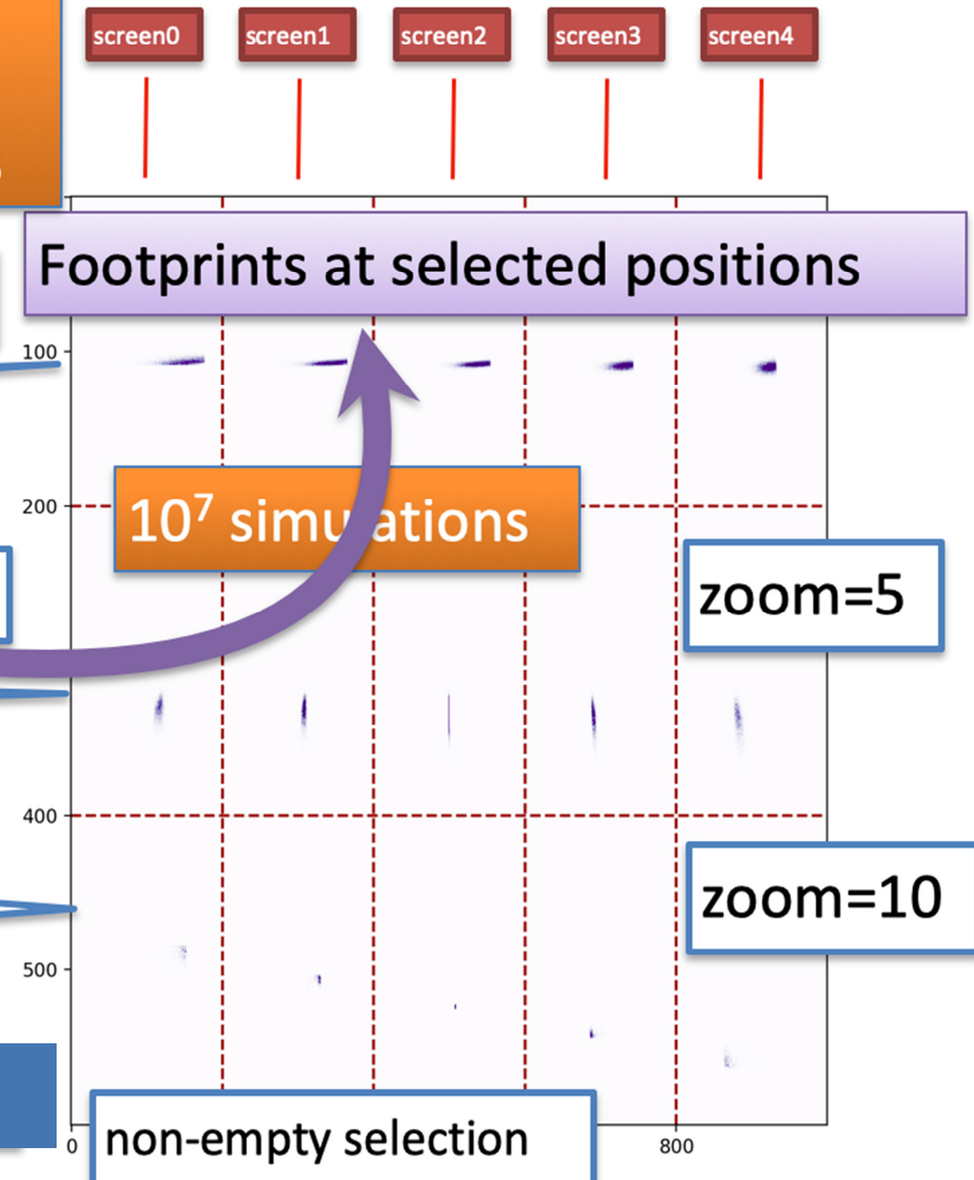


Footprints at selected positions

10^7 simulations

zoom=5

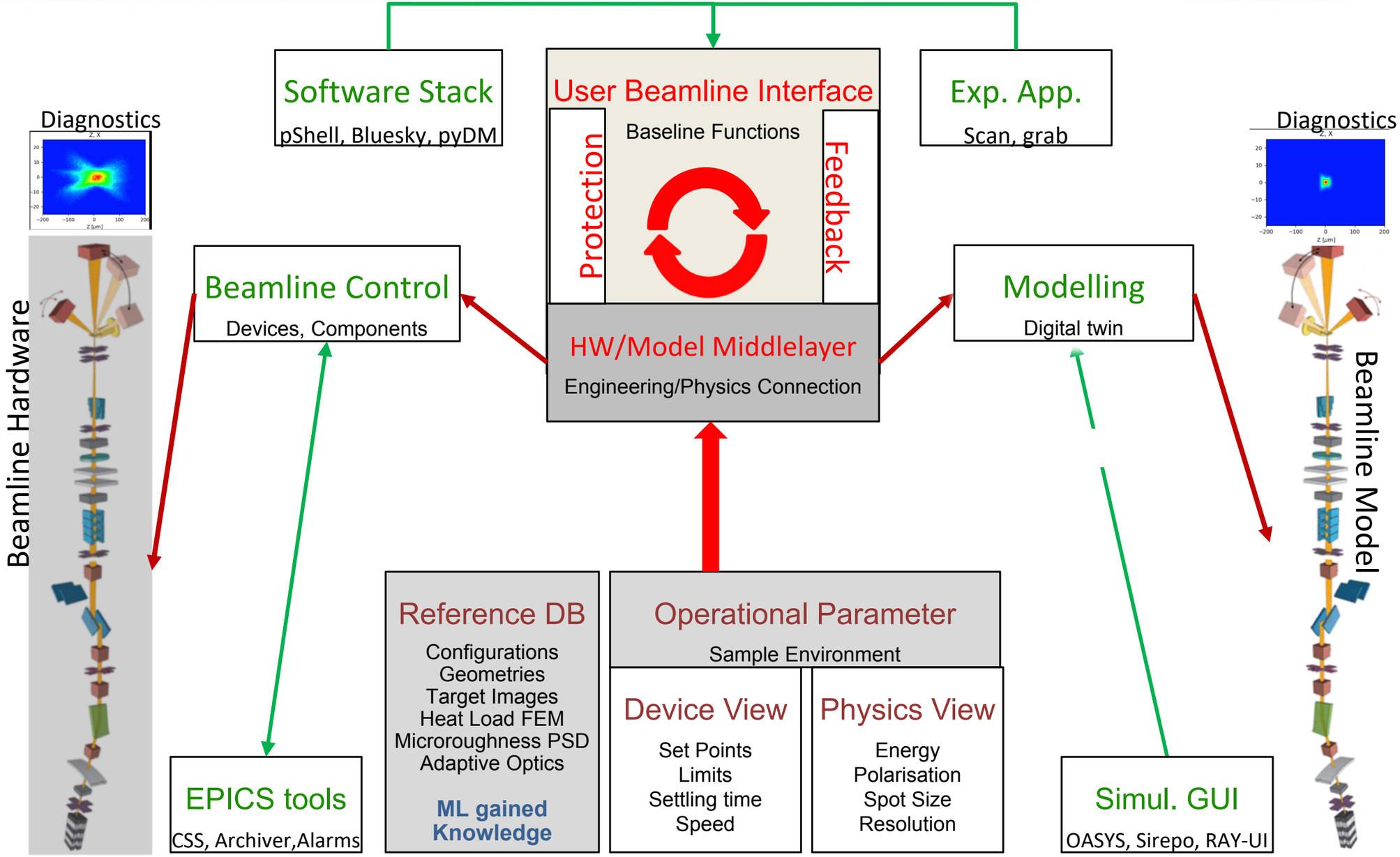
zoom=10

non-empty selection

Derive by machine learning a realistic beamline model

Machine Learning adds Knowledge to Reference DB

- Add trained data gained from experiments



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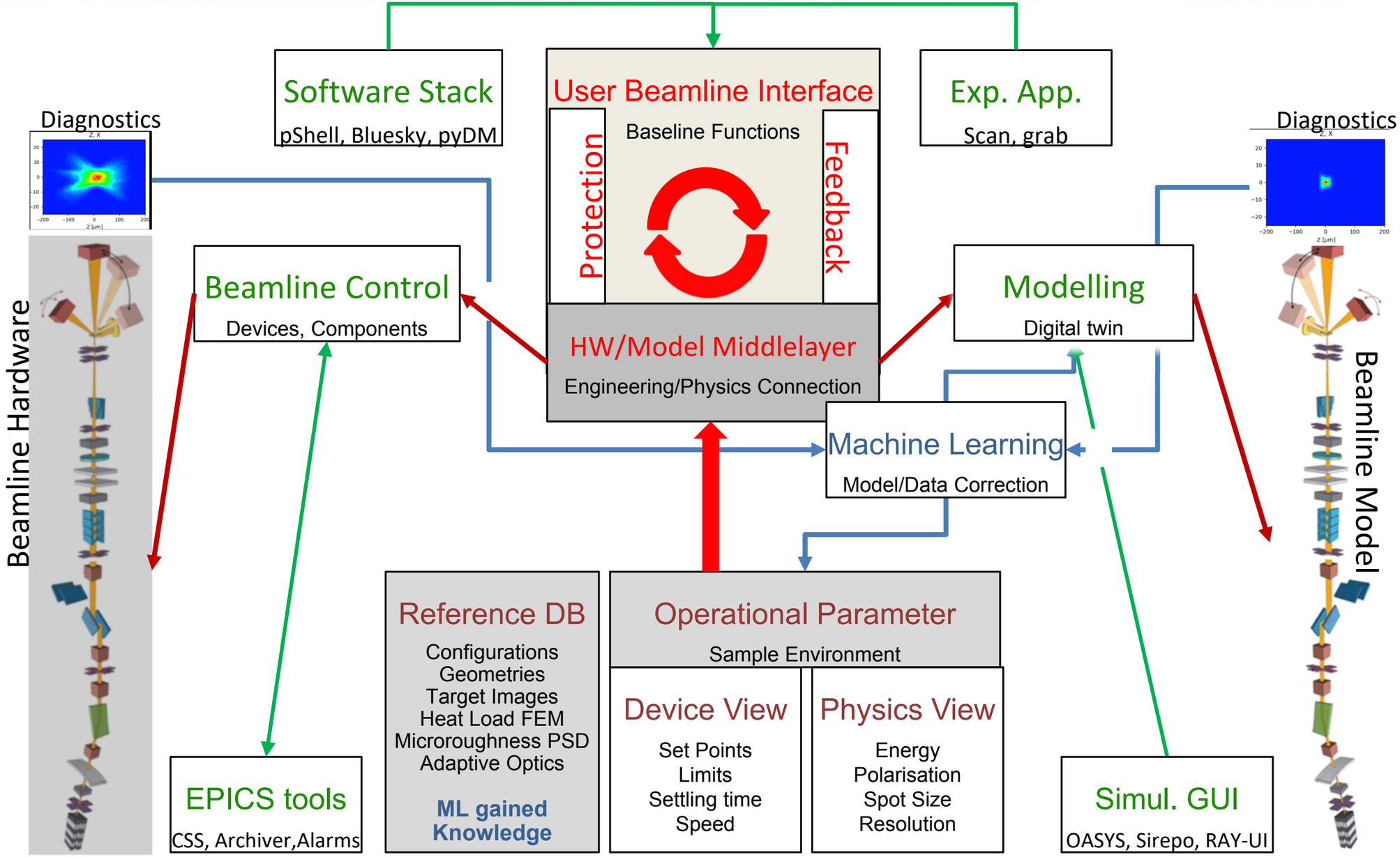
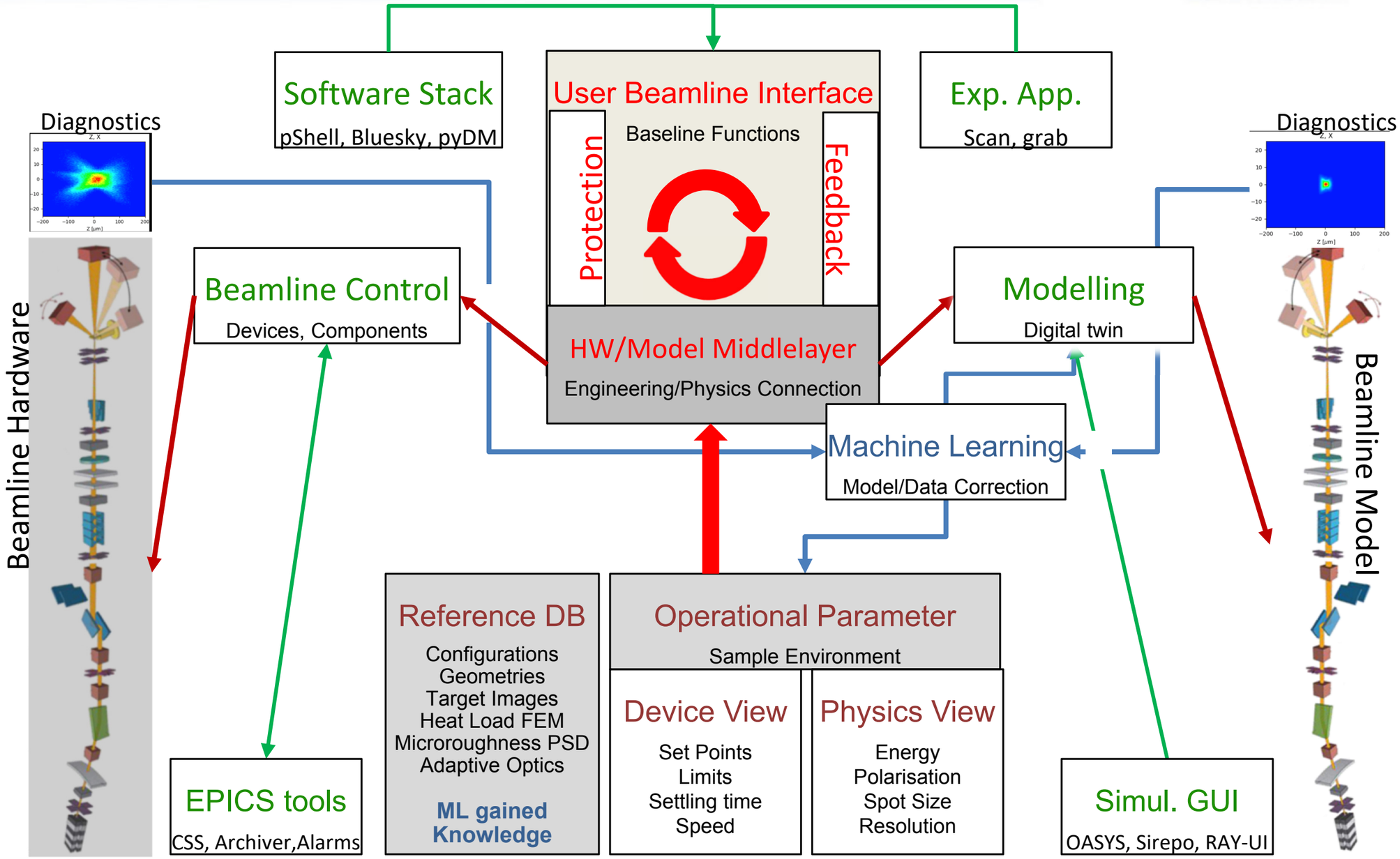


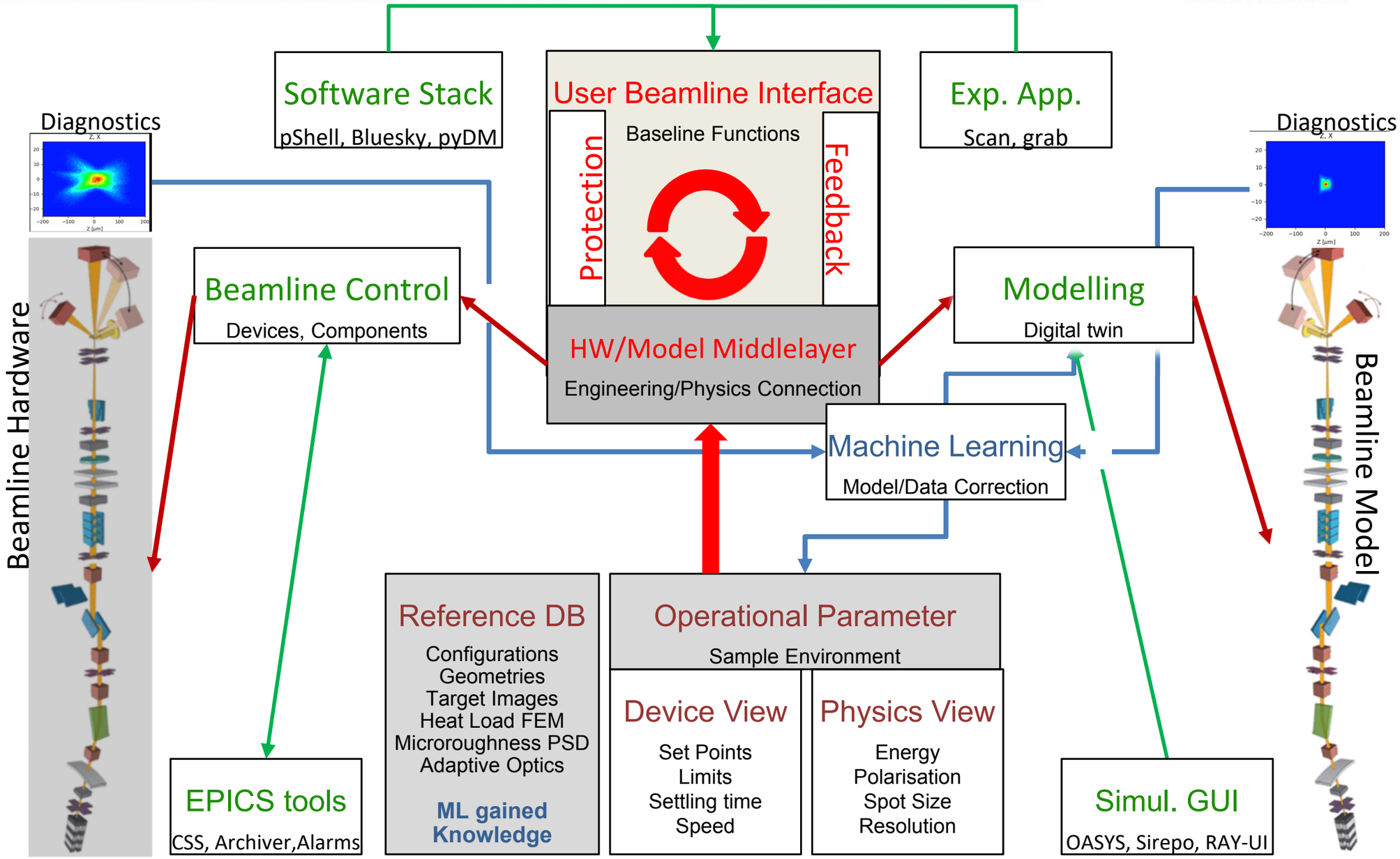
Machine Learning adds Knowledge to Reference DB

- Add trained data gained from experiments
- Put ML derived realistic beamline model into reference repository



Machine Learning adds Knowledge to Reference DB

- Add trained data gained from experiments
- Put ML derived realistic beamline model into reference repository
- Apply to realistic performance analysis



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Beyond Software Solutions – Timing requirements

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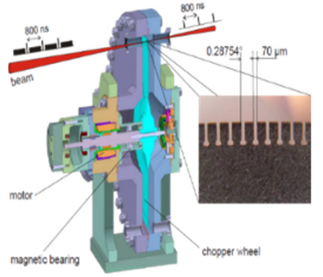
Strong community doing SR timing experiments

- Fancy combination of special bunches and dark gap
- Mechanical chopper isolate single bunches
- Horizontal bunch excitation (PPRE) allow for multi-bunch suppression
- Slicing with fs-laser generates ultra short X-rays and THz

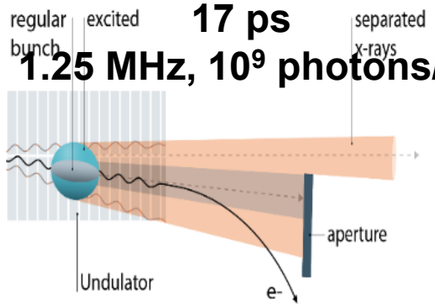
17 ps
1.25 MHz, 10^{13} photons/s



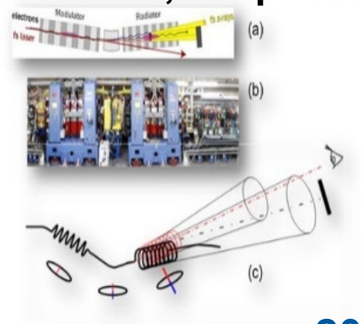
Novel BESSY VSR (Variable pulse length SR)

- Best performance: no dark gap, low and high bunch currents
- Easy accessible via photon sorting, counting
- For others TRIBs (Transversal Resonant Island Buckets) development
  - 1 core, 3 island simultaneously fillable
  - Source points separated by a few 100 µrad
  - Beamline acceptance and readjustment

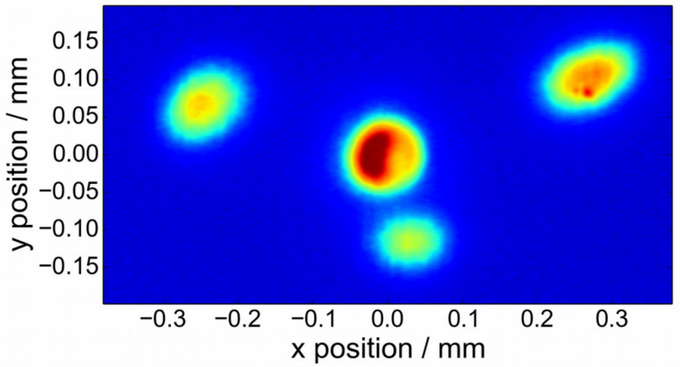
17 ps
1.25 MHz, 10^{9} photons/s



100 fs
6 kHz, 10^{6} photons/s

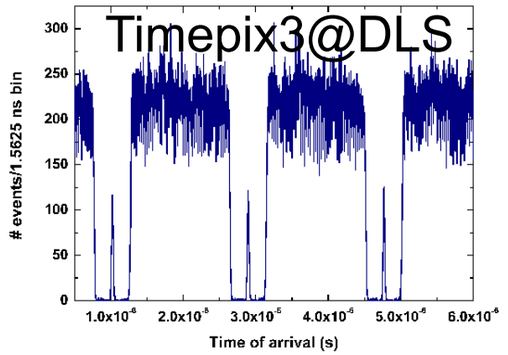


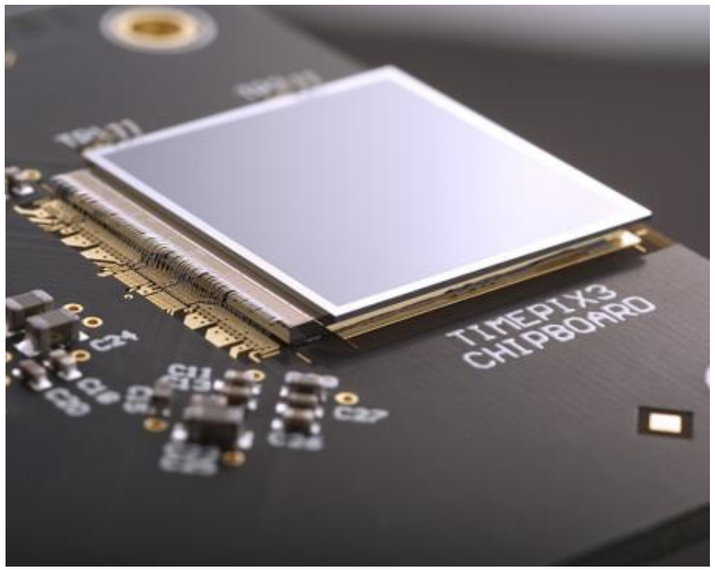
Brainstorming on BESSY III requirements



Other Challenges – Data Streams, Spacial Precision

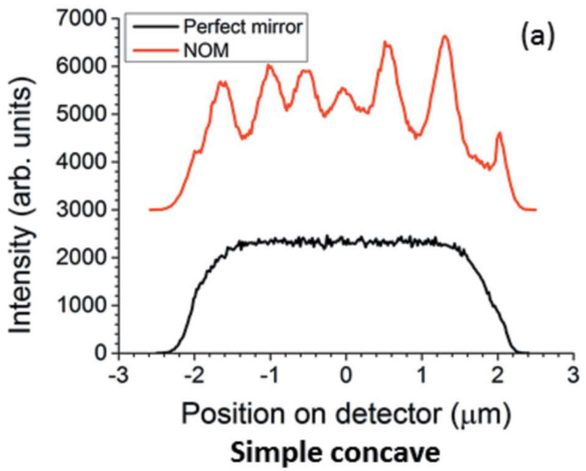
- **Integration of high speed detectors**
- synchronized to the mechatronic environment
- Timepix3 at SPEEM (UE49-PGM)
  4 chips, 512 x 512 effective pixels,
  1.56 ns time resolution,
  120 Mevents/s





- Smaller foci (µm to nm)

- "Tailored" illumination (e.g. flat top)
  with adaptive optics
  (e.g. bi-morph mirrors)

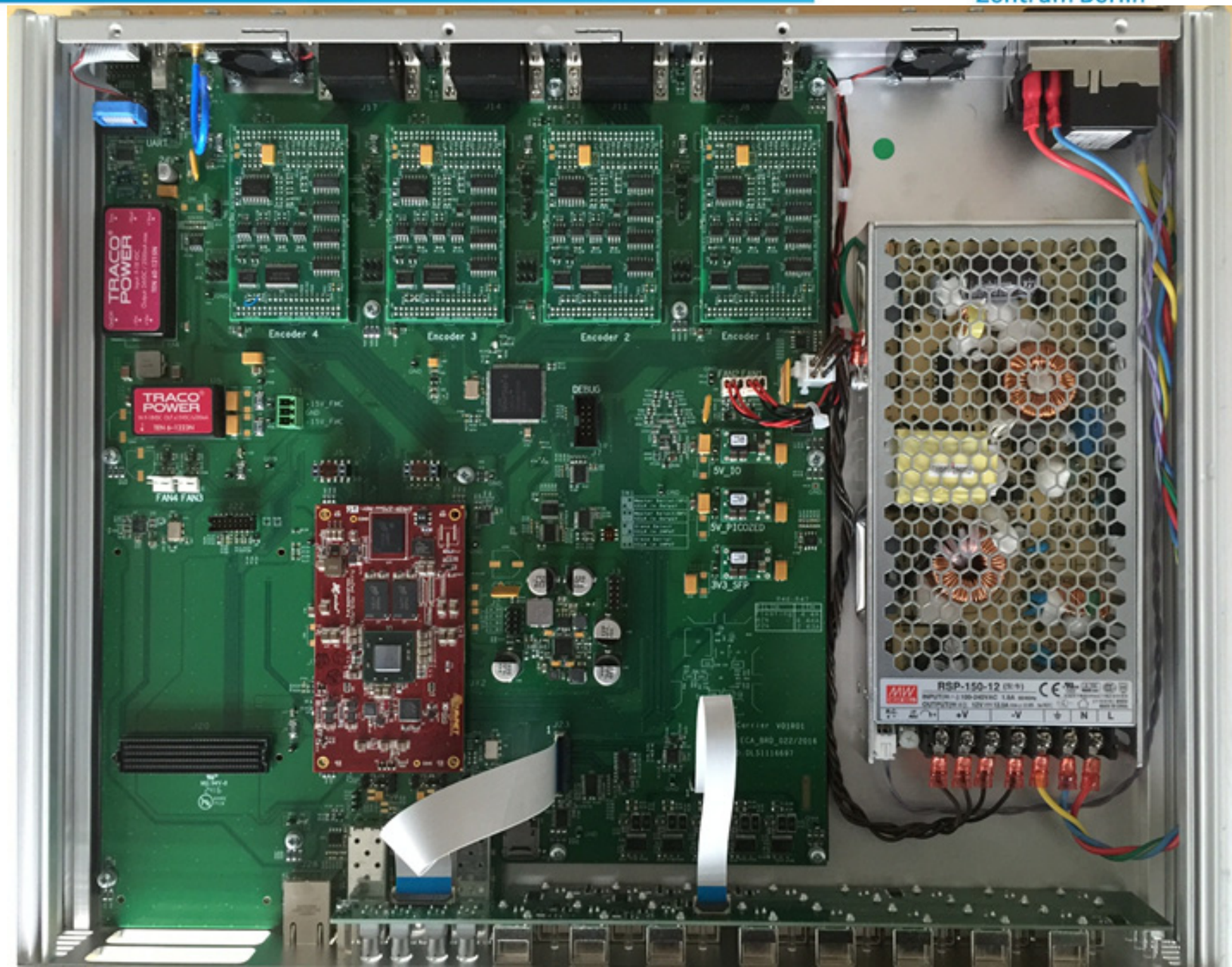


J. P. Sutter *et al.*
JSR **23** (2016) 1333

Beyond Software Solutions - FPGA Based Synchronization

HZB Helmholtz Zentrum Berlin

- Software: solution for low requirements, Sardana continuous scan
- Needs: good + flexible integration of high speed detectors synchronized to the mechatronic environment of the experiments.
- Programmable hardware (FPGA): for high performance, e.g. Panda, Rythm

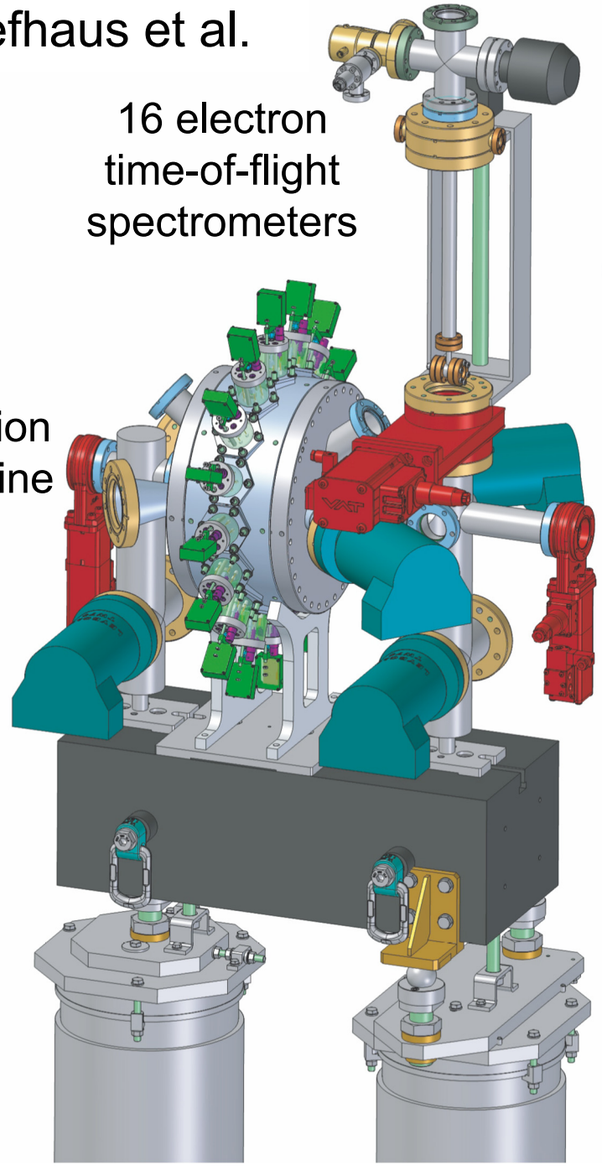


indico.helmholtz-berlin.de/conferenceDisplay.py?confId=11

Novel Photon Diagnostics let you Know Where You Are

J. Viefhaus et al.

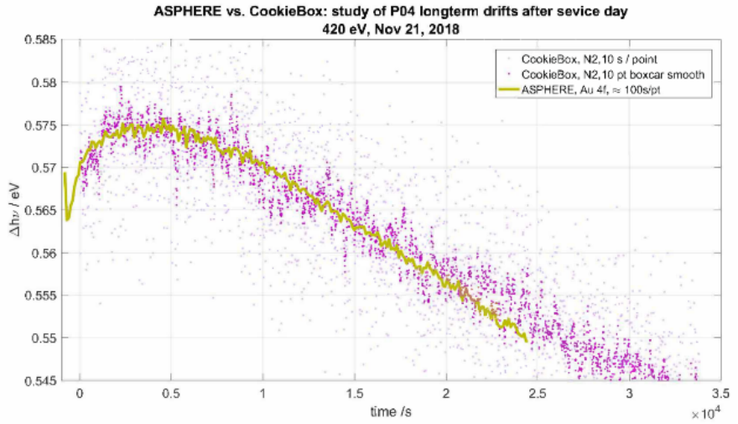
16 electron time-of-flight spectrometers



Connection to beamline

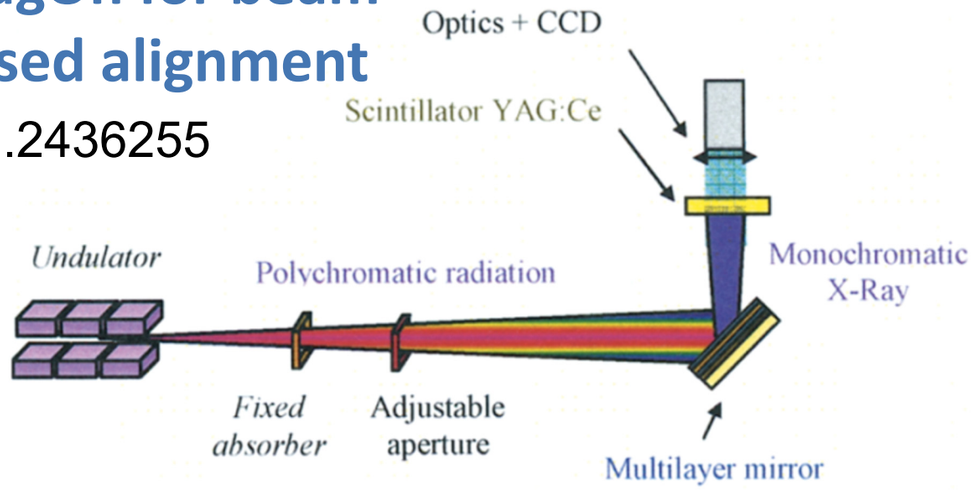
Online Energy, Polarisation

User experiment

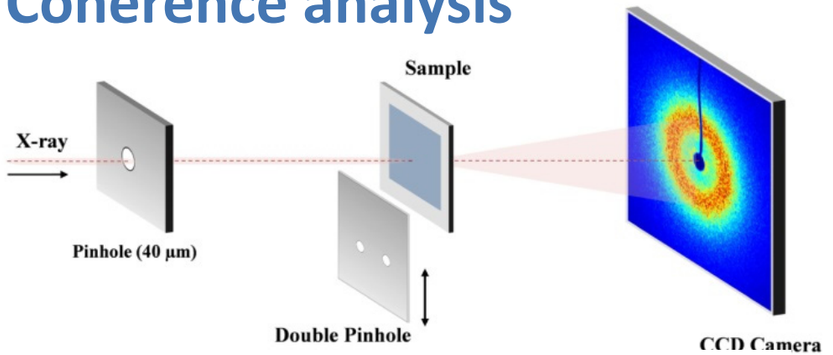


DiagOn for beam based alignment

K. Desjardins et al., https://doi.org/10.1063/1.2436255



Coherence analysis

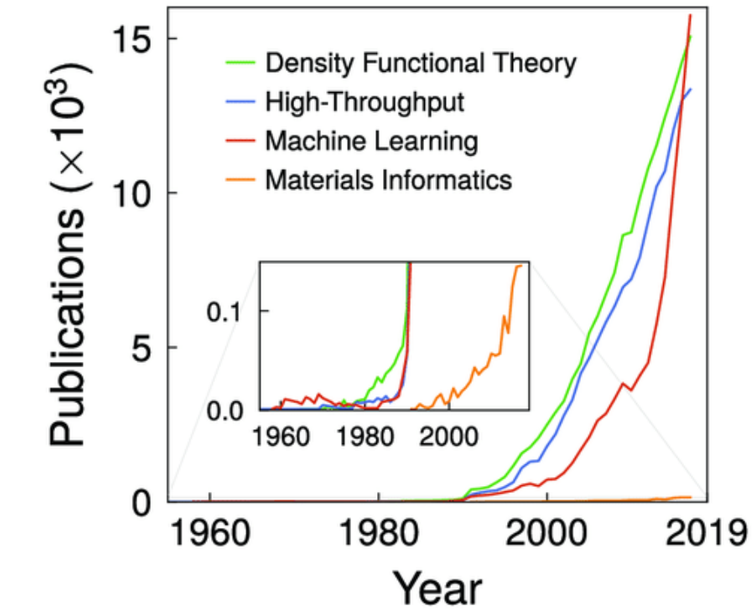


← K. Bagschik *et al.* OE **24** (2016) 23162 + SRI 2018

FAIR Data: enabling the 4th paradigm of science

- For the BESSY material science users the consortium FAIRmat helps scientists to make data Findable, Accessible, Interoperable, and Re-purposable (FAIR).

- The project NOMAD within FAIRmat has already made good progress along the fourth paradigm of science.



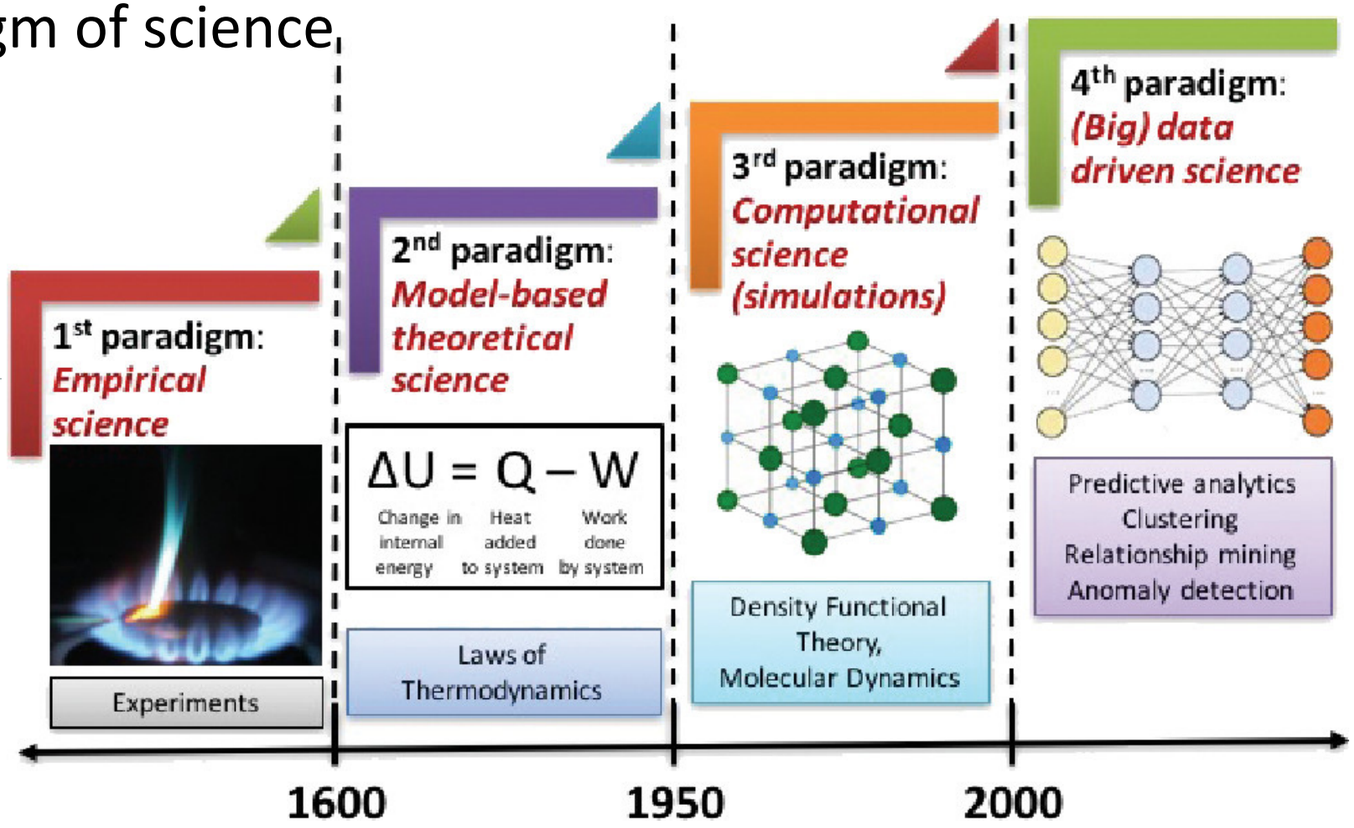


FIG. 1. The four paradigms of science: empirical, theoretical, computational, and data-driven.

Published in: Ankit Agrawal; Alok Choudhary; *APL Materials* **4,** 053208 (2016)

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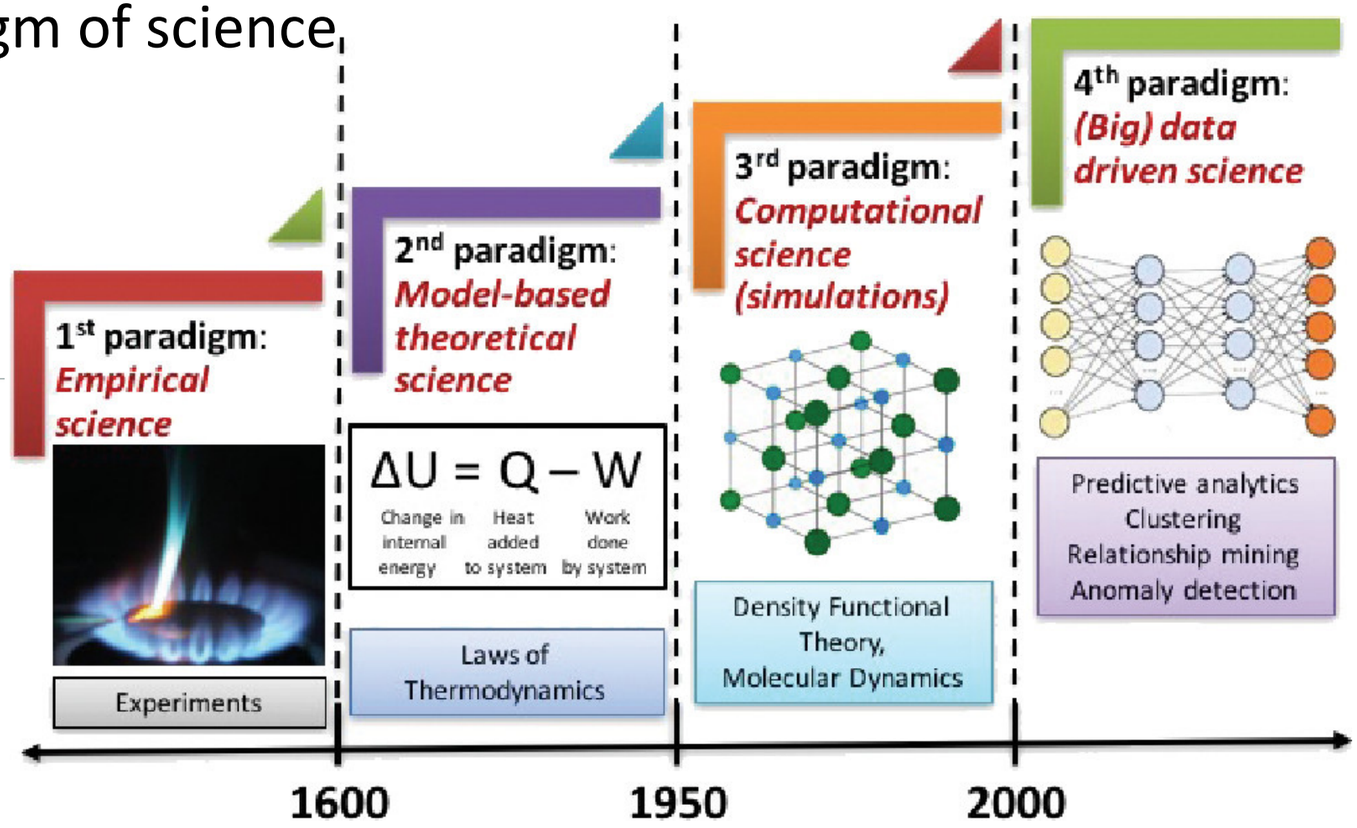
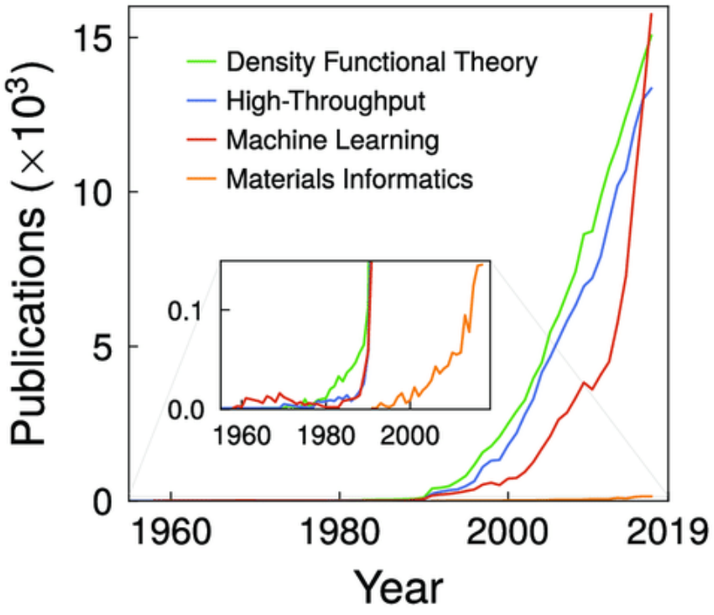


FIG. 1. The four paradigms of science: empirical, theoretical, computational, and data-driven.

Meta-data: common dataset (accelerator, beamline, instrument) describing facility conditions of the experiment.



Published in: Ankit Agrawal; Alok Choudhary; *APL Materials* **4,** 053208 (2016)

After All: Don´t Forget the User Baseline Requirements

Repeated requests and wishes:

- Speedy, reliable network access for remote experiment participation
- Easy scripting, *“dry run”* testing capabilities
- Better robotic support

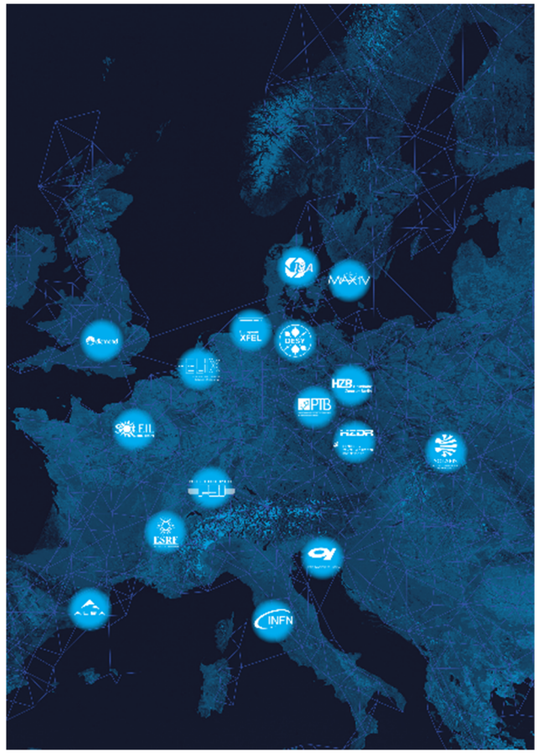
General facility performance metrics

- Accelerator: beam availability, MTBF – online available @ BESSY
- User service: QMS ISO 9001:2015 – BESSY is certified
- Optimized experimental use time – in the works
  - Photons on sample
  - Set-up ready and functioning
  - Data taking feasible
  - Data quality control active
  - ….

Community environment – LEAPS

HZB Helmholtz Zentrum Berlin

LEAPS League of European Accelerator-based Photon Sources



European accelerator based photon sources join their efforts

- Smart specialization
- Accelerators develop and push their specific expertise:

  emittance, coherence, intensity, energy range, pulse length
- Cutting edge experiments find their facility
- Multi-modal experiments span facilities

Tailor beamline and experiment control along international user needs:

- User experience of the IT support should be comparable
- “Common” environments (e.g. similar to MX beamlines)

Summary, Outlook

- Modernization of data taking at BESSY is a long way to go
  - World class instruments generate outstanding results
  - Must not be affected by general upgrade activities.
  - a sustainable data acquisition framework needs to be put in place.

- We have a clear vision, that should help to agree on the goals.
  - Integration of modelling and machine learning
  - Handling of large data streams
  - hardware triggered scanning
  - automation tools for efficient use of beamtime
  - data quality assurance via „near realtime analysis“.

- Within the League of European Accelerator based Photon Sources (LEAPS)
  - user experience of controls and IT support should be comparable

- A complete „digital scientific workflow“ is at a very far horizon.