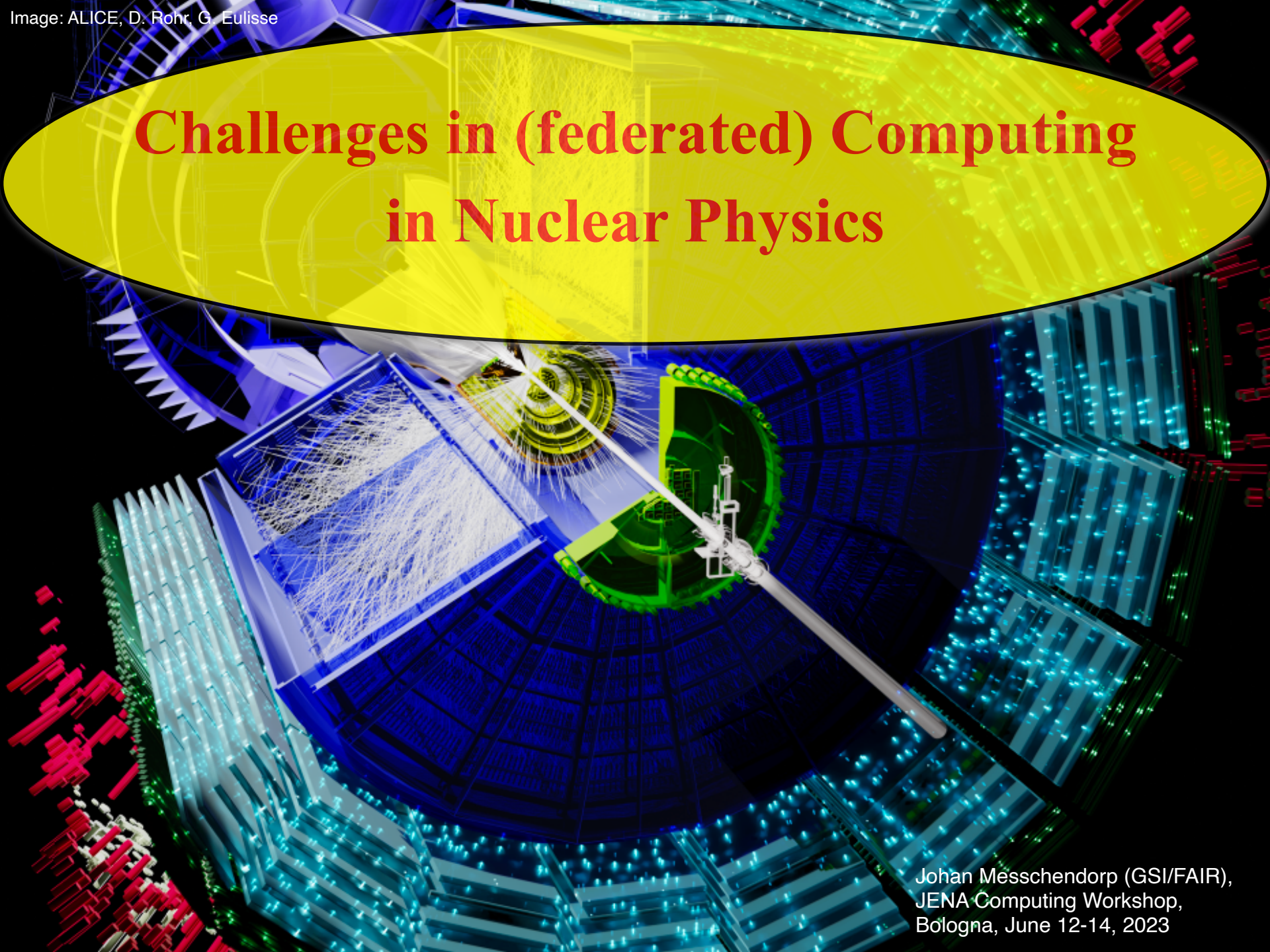
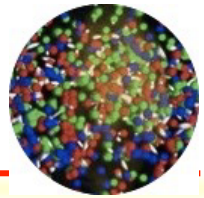


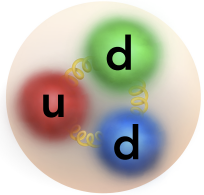
Challenges in (federated) Computing in Nuclear Physics

Johan Messchendorp (GSI/FAIR),
JENA Computing Workshop,
Bologna, June 12-14, 2023

The underlying challenges in a nutshell…



Hot and Dense
Nuclear Matter



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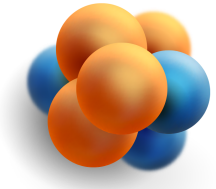
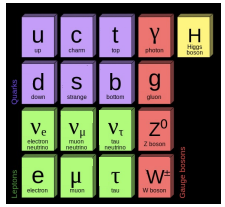


Atomic Nucleus

Nuceli in the Cosmos



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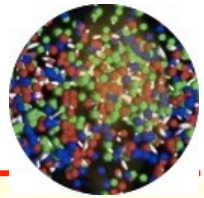

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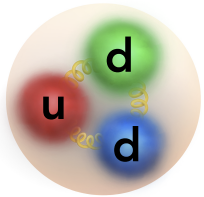

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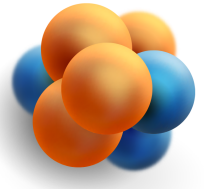

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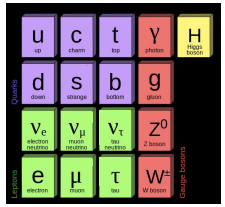

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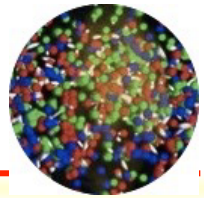

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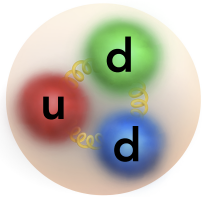

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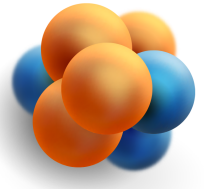

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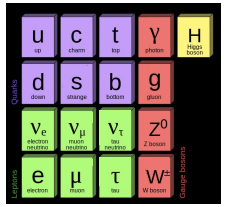

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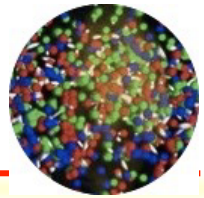

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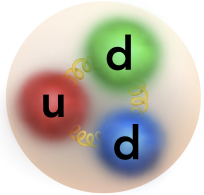

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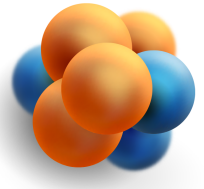

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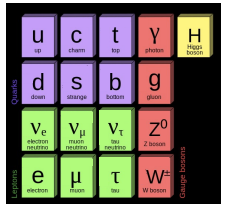

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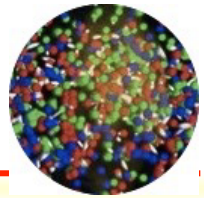

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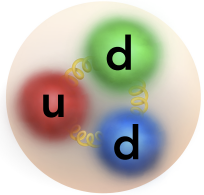

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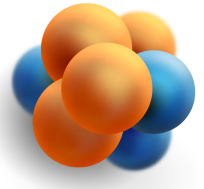

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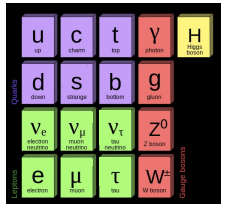

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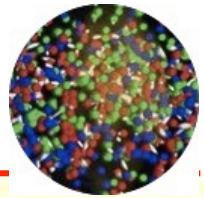
- Computing **support often centrally organised & understaffed compared to HEP** communities!



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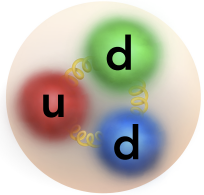

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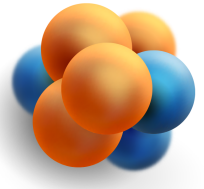

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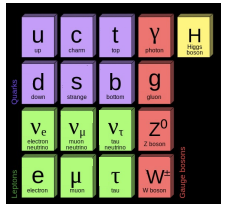

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Facility for Antiproton and Ion Research -
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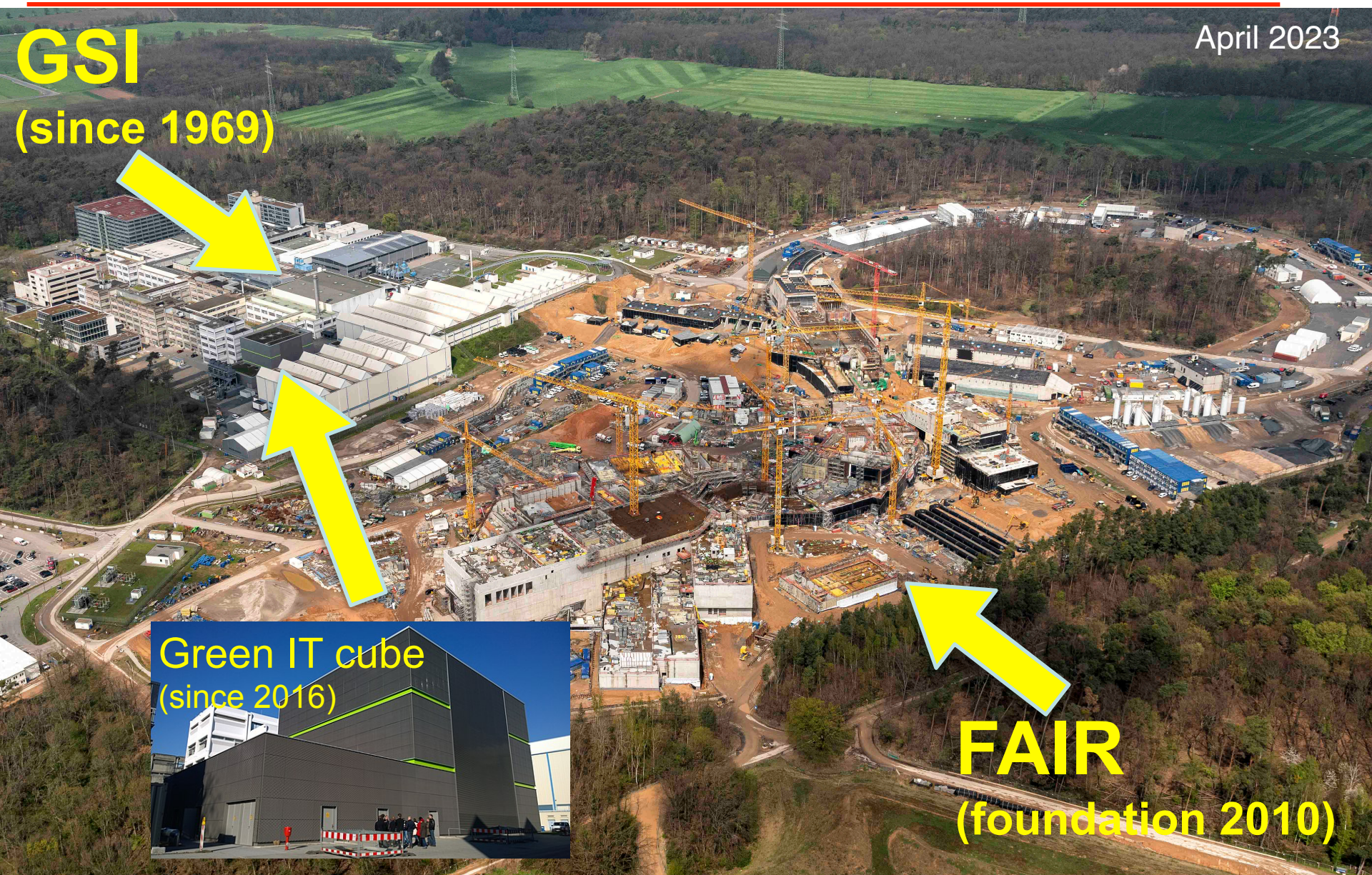

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203x

Cutting-edge science and technology

- ESFRI Landmark near Frankfurt, Germany (ESCAPE)
- Top priority for European Nuclear Physics Community
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- High intensity+precision+diversity+parallel operation
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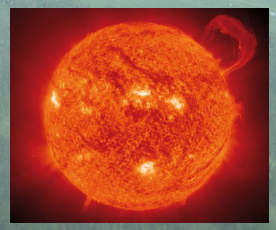
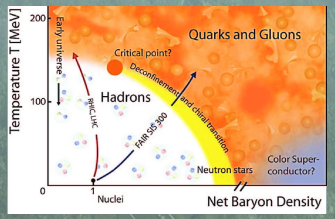
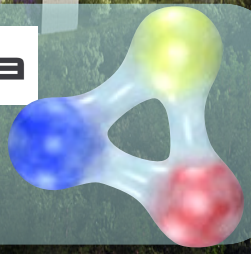
APPA



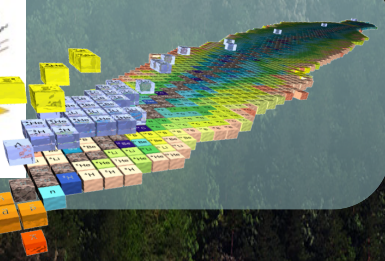
CBM



panda



NUSTAR



+THEORY and BEAM physics

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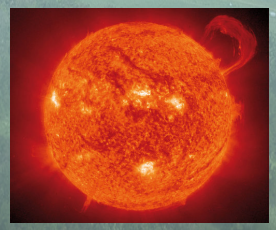

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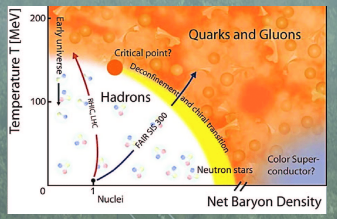

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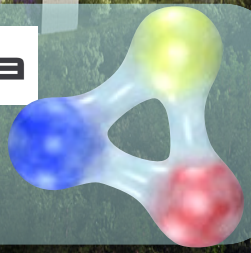

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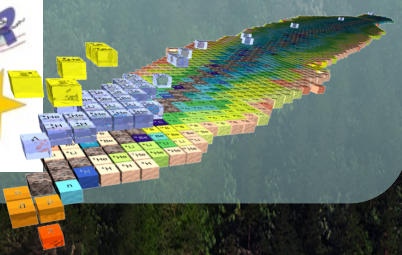

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Towards the next generation "data challenge"

- Volume, Velocity, Veracity, Variety, and Complexity!
- ~TB/s data rates, online processing, ~5×10^5 cores
- Data stored on disk ~35 PB/year
- Distributed computing with a large user community
- Committed to "open-science" (FAIR) concept

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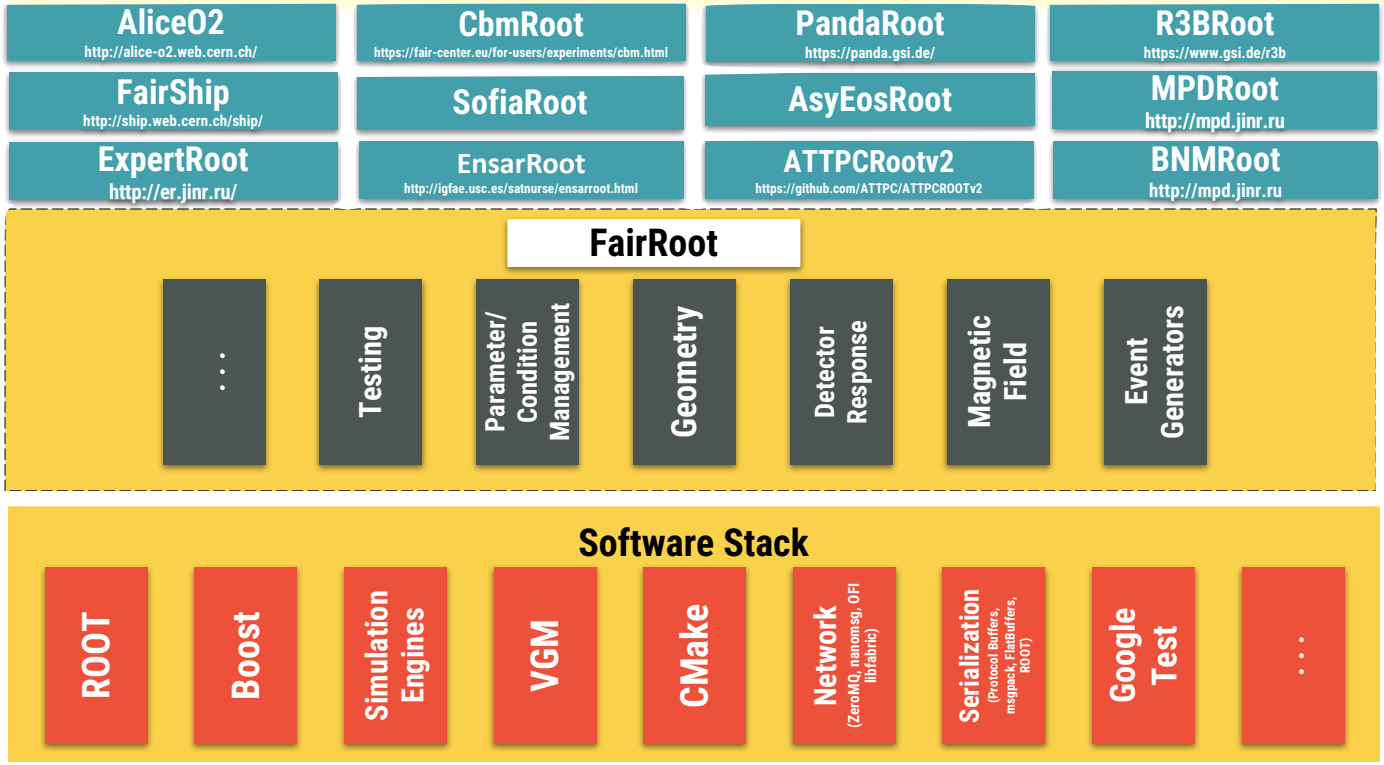
- Integrate computing systems in development with ongoing activities (**learn by experience**).

Example success story - FairRoot

Mohammad Al-Turany et al.



Example success story - FairRoot

Mohammad Al-Turany et al.

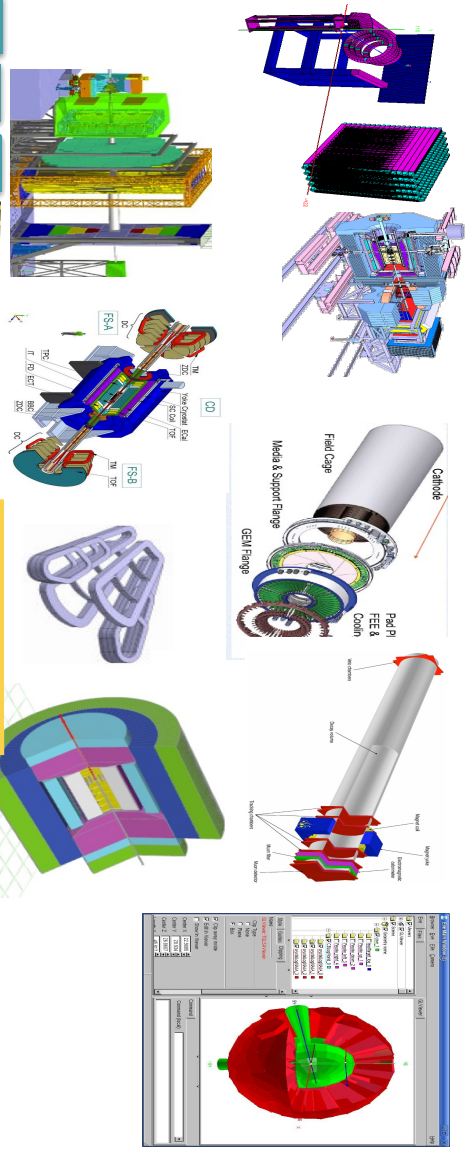
AliceO2 http://alice-o2.web.cern.ch/	**CbmRoot** https://fair-center.eu/for-users/experiments/cbm.html	**PandaRoot** https://panda.gsi.de/	**R3BRoot** https://www.gsi.de/r3b
FairShip http://ship.web.cern.ch/ship/	**SofiaRoot**	**AsyEosRoot**	**MPDRoot** http://mpd.jinr.ru
ExpertRoot http://er.jinr.ru/	**EnsarRoot** http://igfae.usc.es/satnurse/ensarroot.html	**ATTPCRootv2** https://github.com/ATTPC/ATTPCROOTv2	**BNMRoot** http://mpd.jinr.ru

FairRoot

- . . .
- Testing
- Parameter/ Condition Management
- Geometry
- Detector Response
- Magnetic Field
- Event Generators

Software Stack

- ROOT
- Boost
- Simulation Engines
- VGM
- CMake
- Network (ZeroMQ, nanomsg, OFI libfabric)
- Serialization (Protocol Buffers, msgpack, FlatBuffers, ROOT)
- Google Test
- . . .



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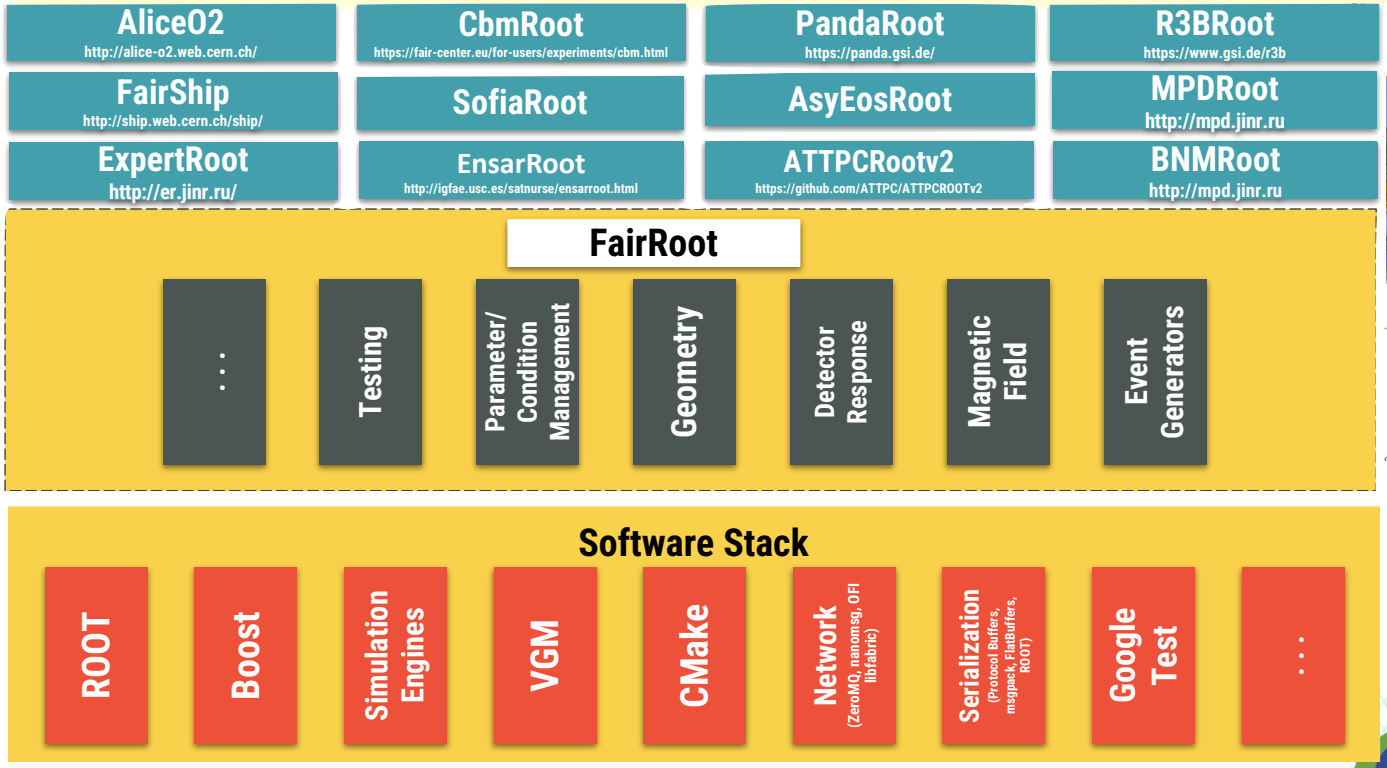

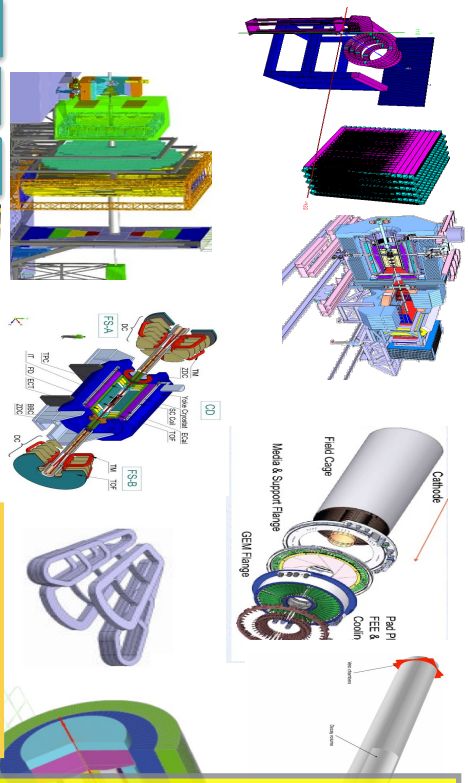

- Used for FAIR design studies, feasibility MC studies, and (Phase-0) experiments!
- Generates lots of synergy between different groups at FAIR and outside FAIR
- Example case for a successful “federated” computing!

Enough challenges still to tackle (and in my view underestimated)

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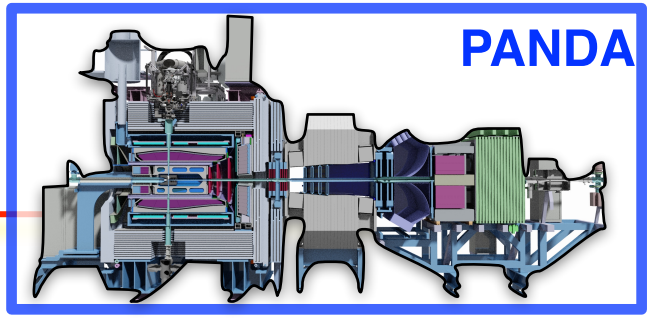

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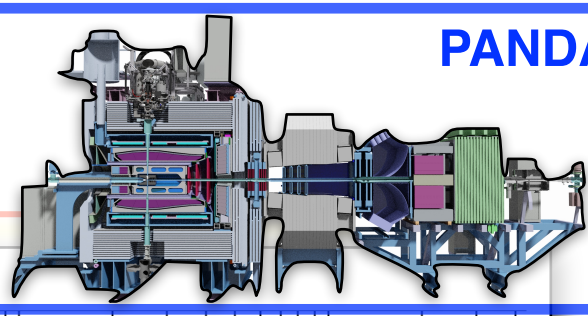
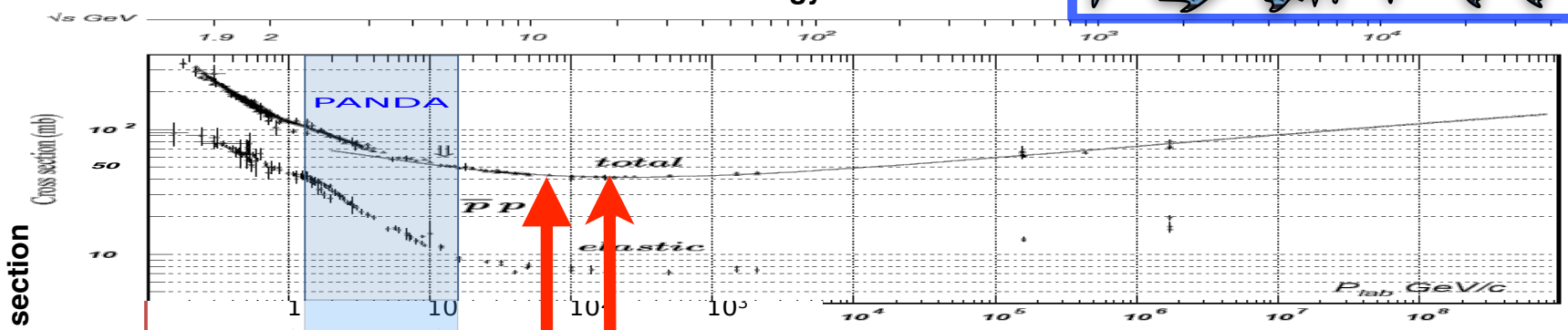


Energy



Cross section

1 mb
100 μb
10 μb
1 μb
100 nb
10 nb
1 nb

1/10.000

1/10.000.000

Glueballs

η_c
χ_{c2}
X(3872)
$\eta_c\pi^0$
χ_{c0}

Hybrids

....finding *many* needles in haystack!
…background similar to signal topology

Free-streaming online data-processing scheme

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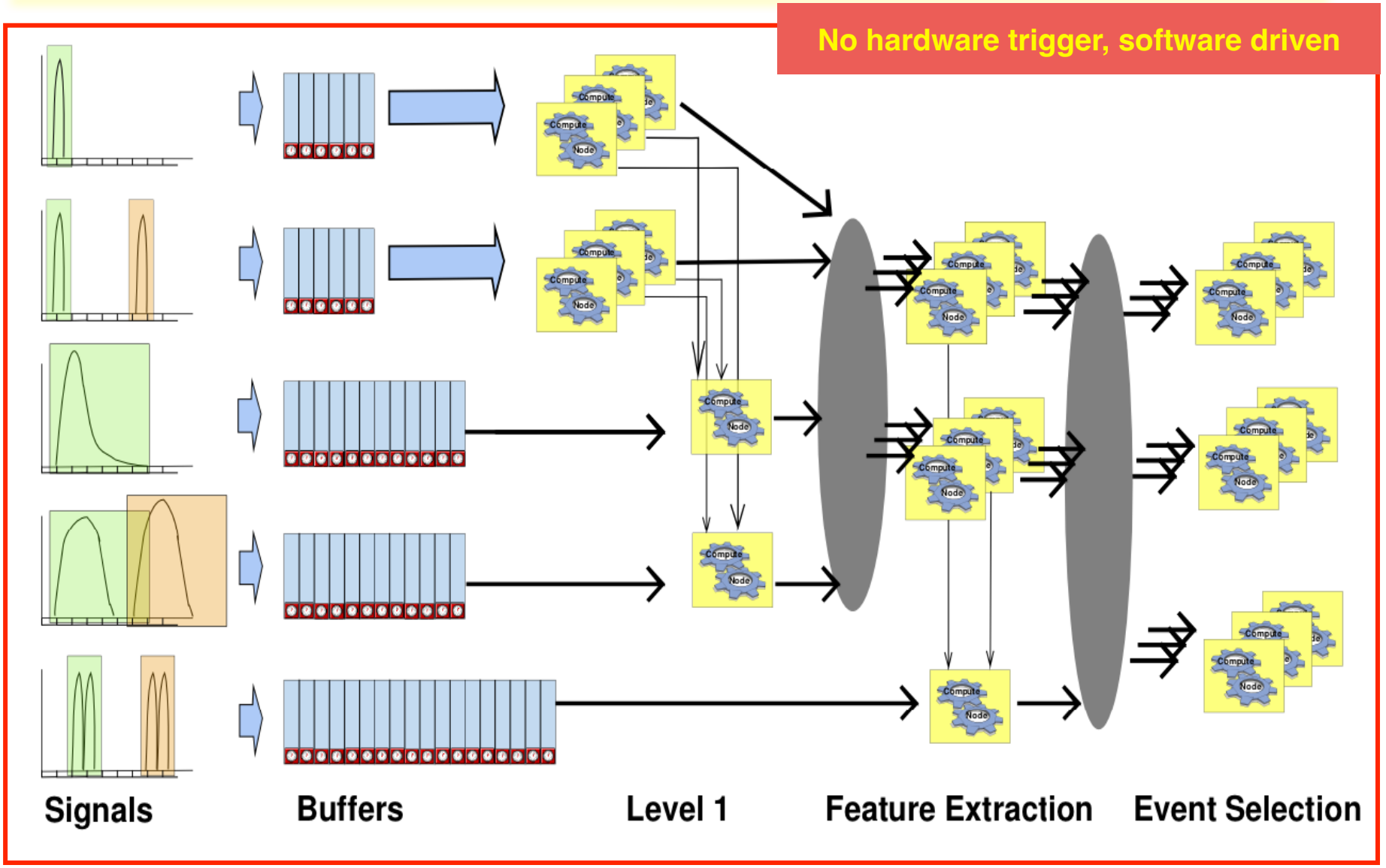
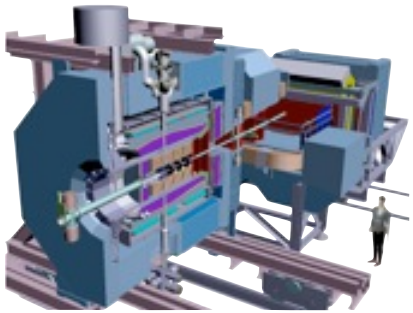


Intelligent *in-situ* data processing



10^7 /s

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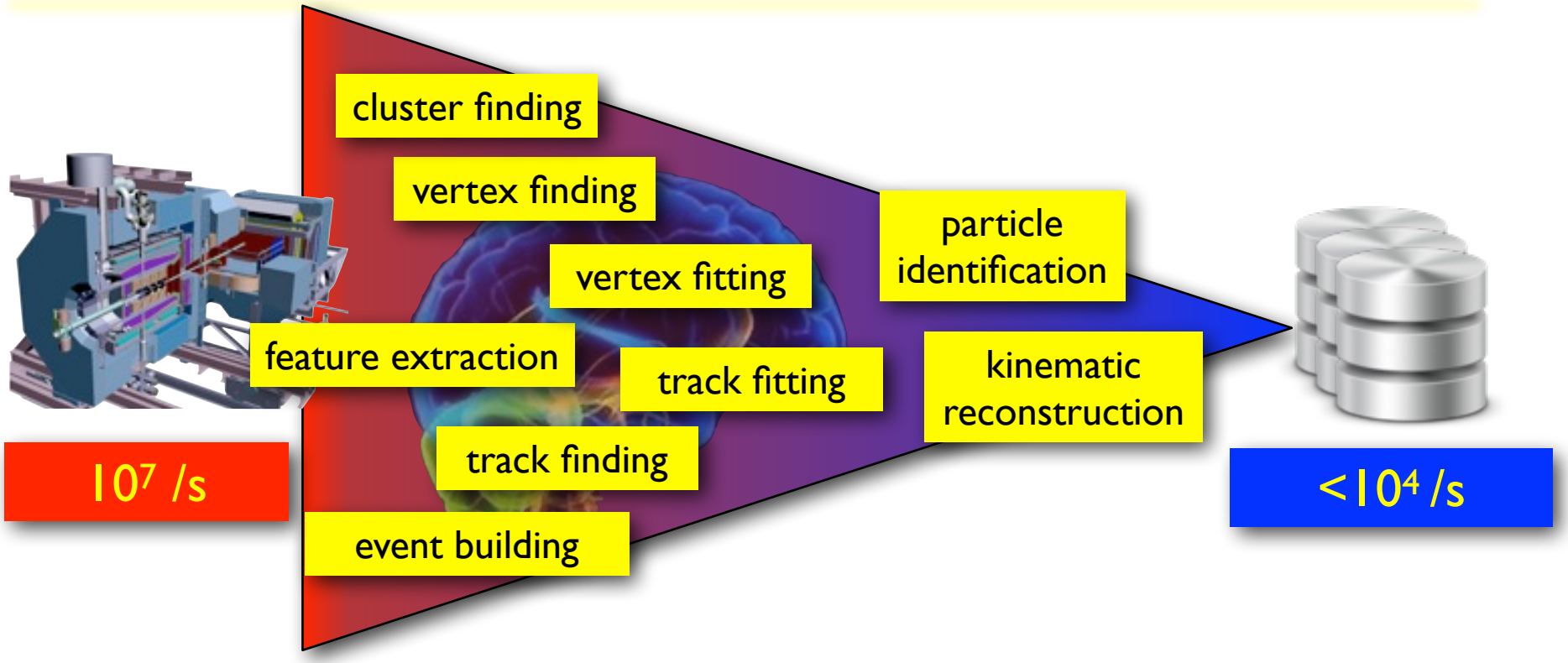
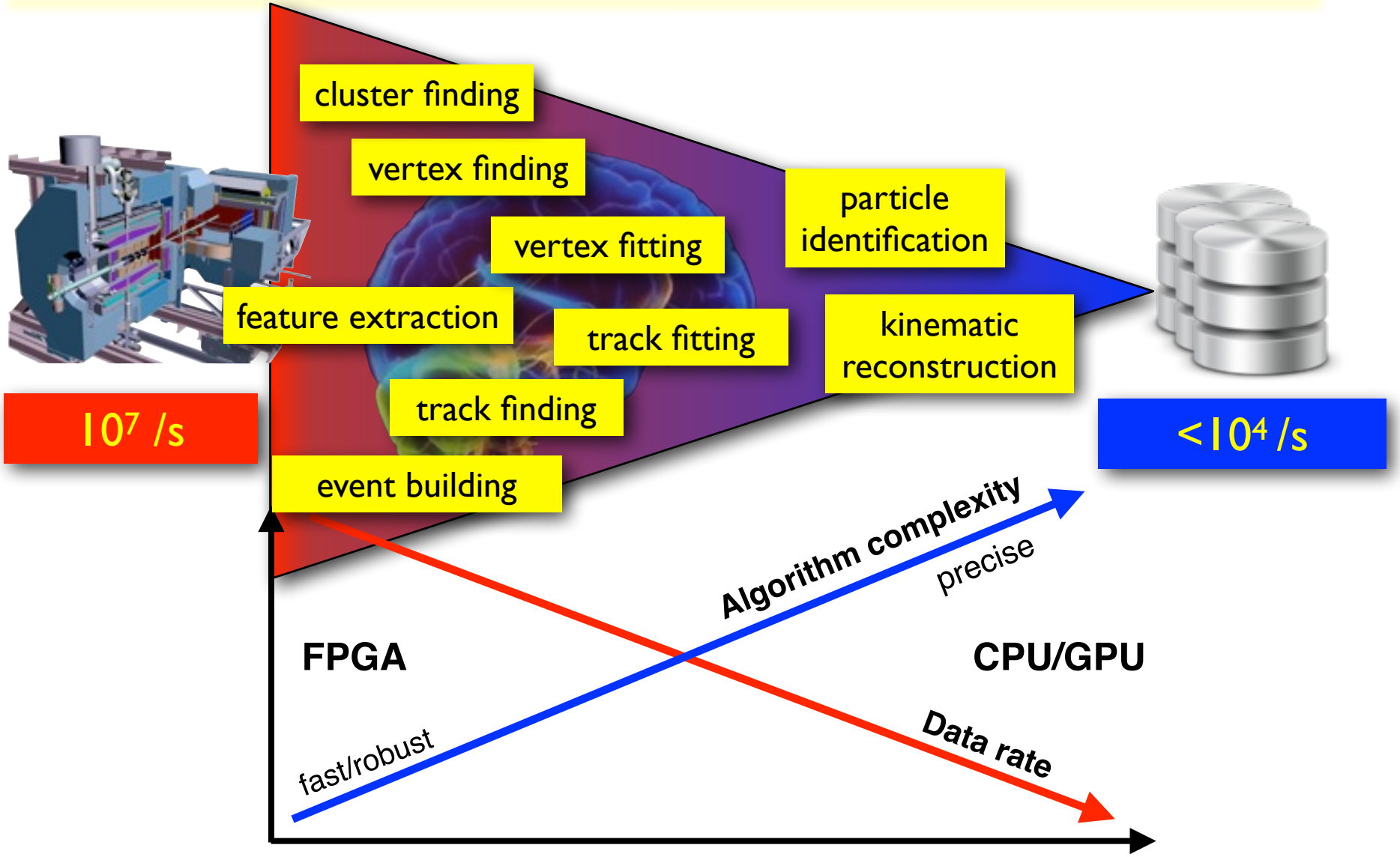


Intelligent *in-situ* data processing



Tackling online-data processing -
a *federated* approach towards a framework

M. Al-Turany et al.

FAIRROOT meets ALICE O^2

Tackling online-data processing -
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FAIRROOT meets ALICE O²

ALICE O²:

- **DAQ, online & offline with one framework**

Tackling online-data processing -
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ALICE O²:

- DAQ, online & offline with one framework

FAIRROOT:

- Concurrency, merging online and offline

Tackling online-data processing -
a *federated* approach towards a framework

M. Al-Turany et al.

FAIRROOT meets ALICE O²

ALICE O²:

- DAQ, online & offline with one framework

+

FAIRROOT:

- Concurrency, merging online and offline

=

ALFA:

- Join forces in a combined framework!

Tackling online-data processing -
a *federated* approach towards a framework

M. Al-Turany et al.

FAIRROOT meets ALICE O²

ALFA

FAIRMQ:

- Based on “actor” model of concurrency
- Asynchronous messaging toolkit
- Broad scala of messaging pattern
- Easy and scalable networking
- Commun. layer: 0MQ, shared memory, and Libfabric

Tackling online-data processing -
a *federated* approach towards a framework

M. Al-Turany et al.

FAIRROOT meets ALICE O²

- BSD sockets API
- Bindings for 30+ languages
- Lockless and Fast
- Automatic re-connection
- Multiplexed I/O

ALFA

FAIRMQ:

- **Based on "actor" model of concurrency**
- **Asynchronous messaging toolkit**
- **Broad scala of messaging pattern**
- **Easy and scalable networking**
- **Commun. layer: 0MQ, shared memory, and Libfabric**

Tackling online-data processing -
a *federated* approach towards a framework

David Rohr, Giulio Eulisse, ALICE

O²: Software Framework

Framework & Data Processing Layer (DPL)

Hides the hiccups of a distributed system, presenting a familiar "Data Flow" system.

- ***Reactive-like design*** *(push data, don't pull)*
- ***Implicit workflow definition*** *via modern C++ API.*
- ***Core common tasks:*** *topological sort of dependencies, deployment of generated topologies, data life handling, service management, common infrastructure services, plug-in manager.*
- ***Integration*** *with the rest of the production system, e.g. Monitoring, Logging, Control.*

Data Layer: O2 Data Model

Message passing aware data model. Support for multiple backends:

- **Simplified, zero-copy** *format optimised for performance and direct GPU usage.*
- **ROOT based serialisation.** *Useful for QA and final results.*
- **Apache Arrow based.** *Backend of the analysis data model and for integrating with other tools.*
- *We contributed the* **RDataFrame Arrow backend to ROOT**.

Transport Layer: ALFA / FairMQ[1]

- **Joint collaboration with FAIR and GSI**
- **Standalone processes (devices)** *for deployment flexibility & resilience*
- **Message passing** *as a parallelism paradigm*
- **Shared memory** *backend for reduced memory usage and improved performance*
- **Seamless remote** communication

Tackling online-data processing -
a *federated* approach towards a framework

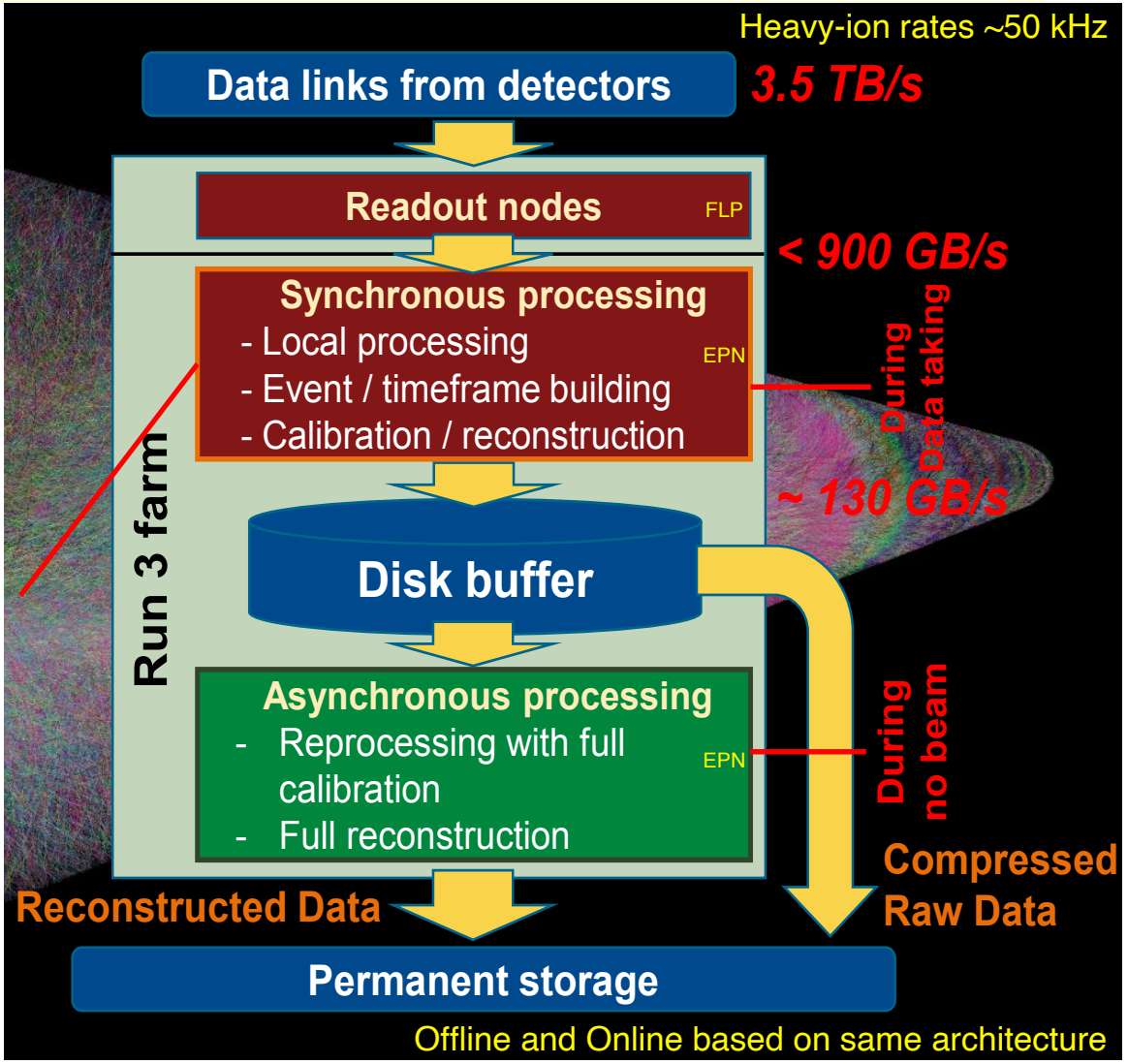
David Rohr, Giulio Eulisse, ALICE

O²: Software Framework

Framework &
Data Processing Layer (DPL)

Data Layer: O2 Data Model

Transport Layer: ALFA / FairMQ[1]



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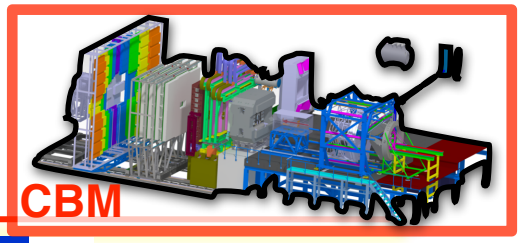
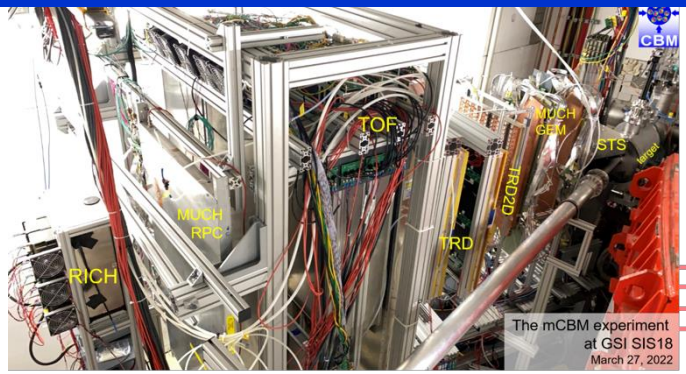
a *federated* approach towards a framework



The free-streaming CBM DAQ and data processing

N.Herrmann, CBM



optical fibers 50m

DAQ container

CRI (PCIe) @ FLES entry nodes

optical fibers 300 m

FLES processing nodes

FAIR Phase 0 Research Program

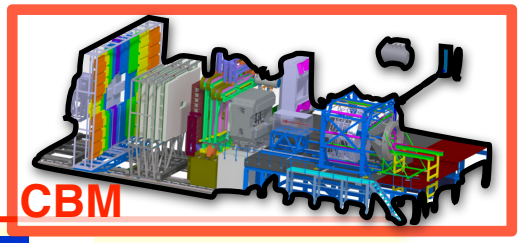
TFC (CRI based)

triggerless-streaming FEE **assigning time stamps to hits**

1 m Copper → GBTx → 50 m optical → CRI FPGA **µSlice building** FLES entry nodes → 300 m optical InfiniBand → Green IT Cube

Timeslice Building
Event Reconstruction
Event Selection
Archiving

Tackling online-data processing -
a *federated* approach towards a framework



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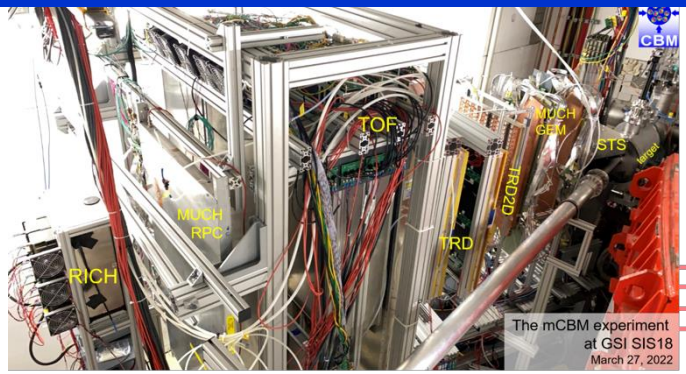

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Timeslice Building
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TFC (CRI based)

triggerless-streaming FEE **assigning time stamps to hits**

1 m Copper

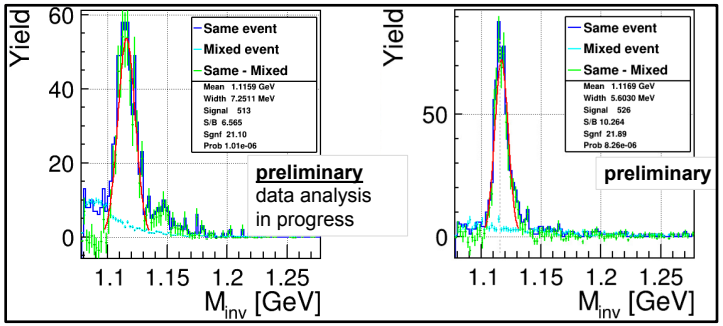
GBTx

50 m optical

CRI FPGA **µSlice building** FLES entry nodes

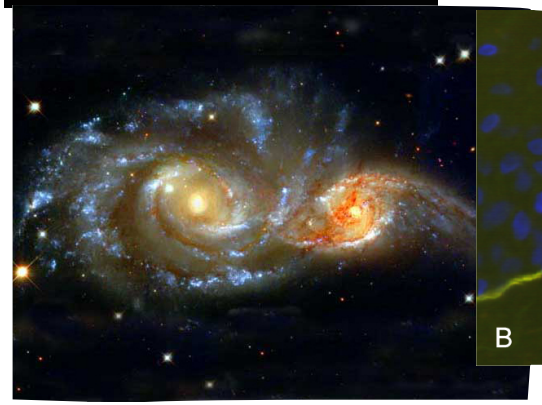
300 m optical InfiniBand

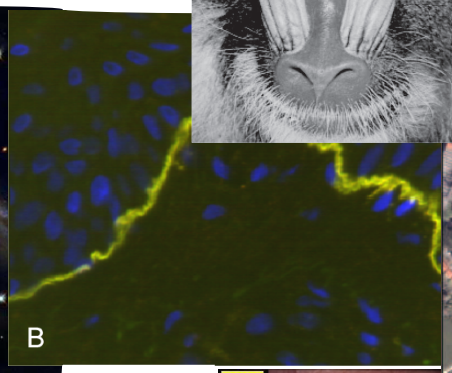
run 2188, March 31, 03:15 CET,
10^7 U ions per spill, approx. 100 kHz averaged collision rate
Applied
filter condition: 1 T0 hit, 2 STS hits, 5 TOF hits ("Λ trigger")

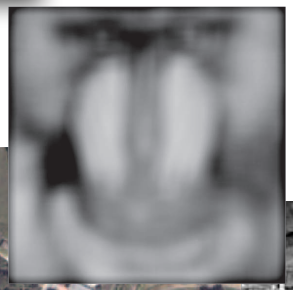


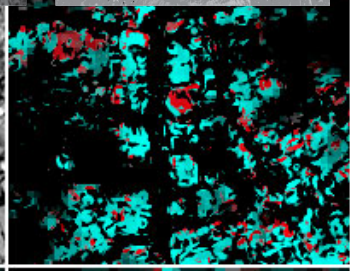
Towards "smarter" algorithms

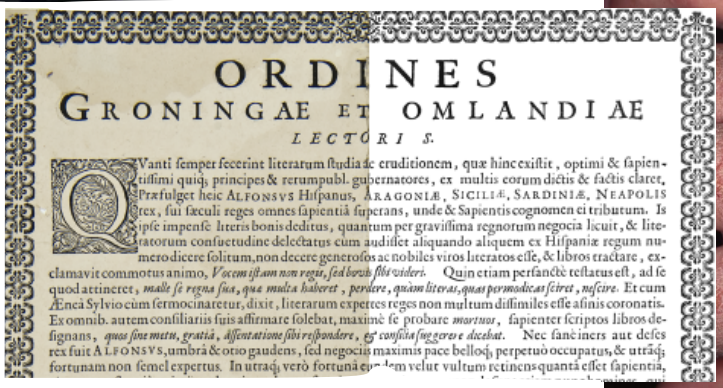
Computer Vision
Machine Learning
Artificial Intelligence

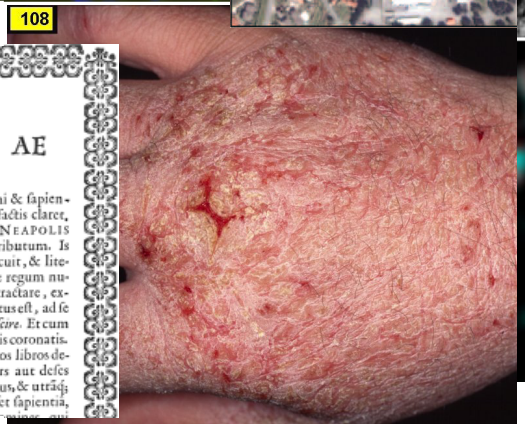


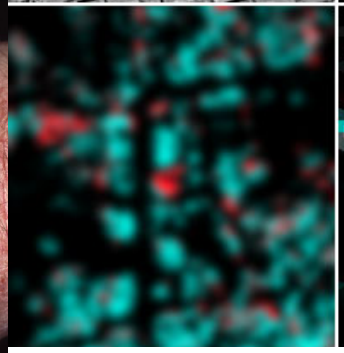


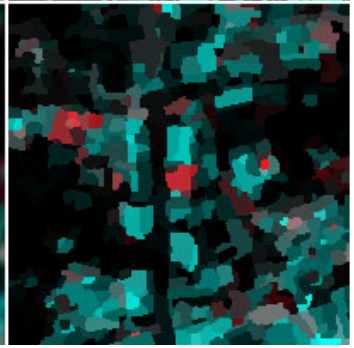








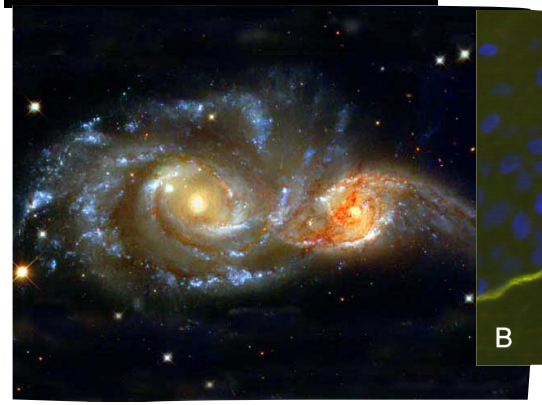


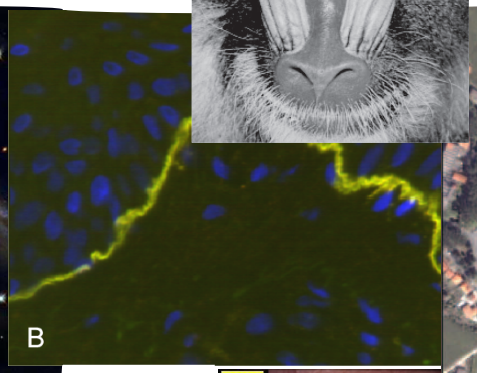


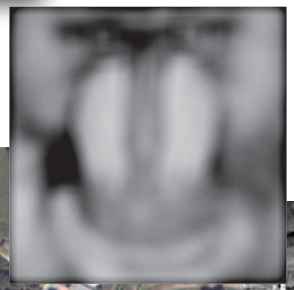
Towards "smarter" algorithms

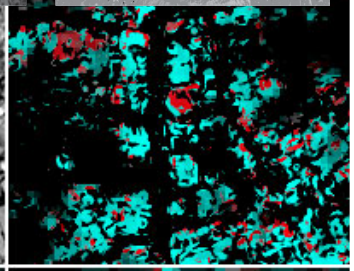
Computer Vision
Machine Learning
Artificial Intelligence

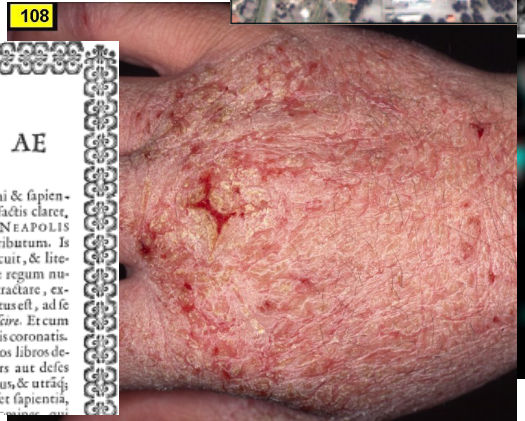
- Image filtering techniques
- Novel cluster finders
- Statistical pattern recognition
- Deep neural networks

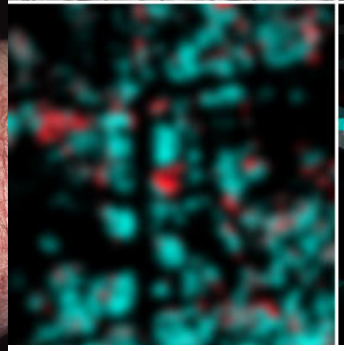


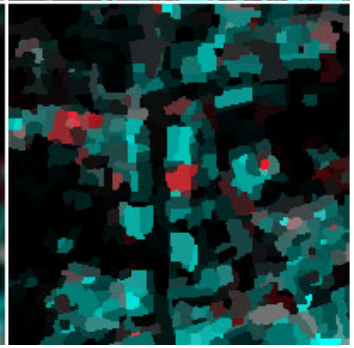






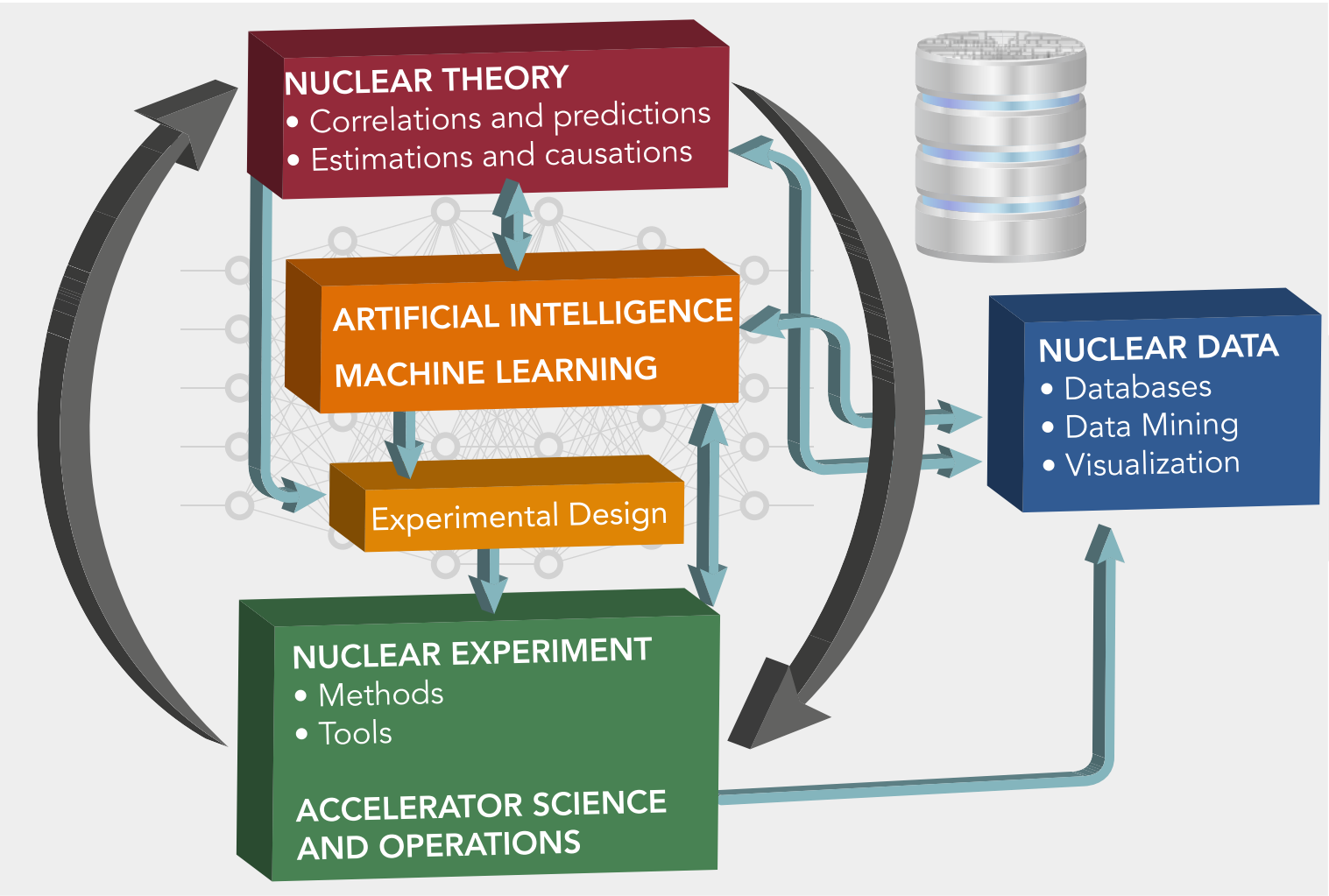






Role of ML and AI in nuclear physics

"Machine Learning in Nuclear Physics",
Bohnlein, Diefenthaler, Sato, Schram, arXiv:2112.02309



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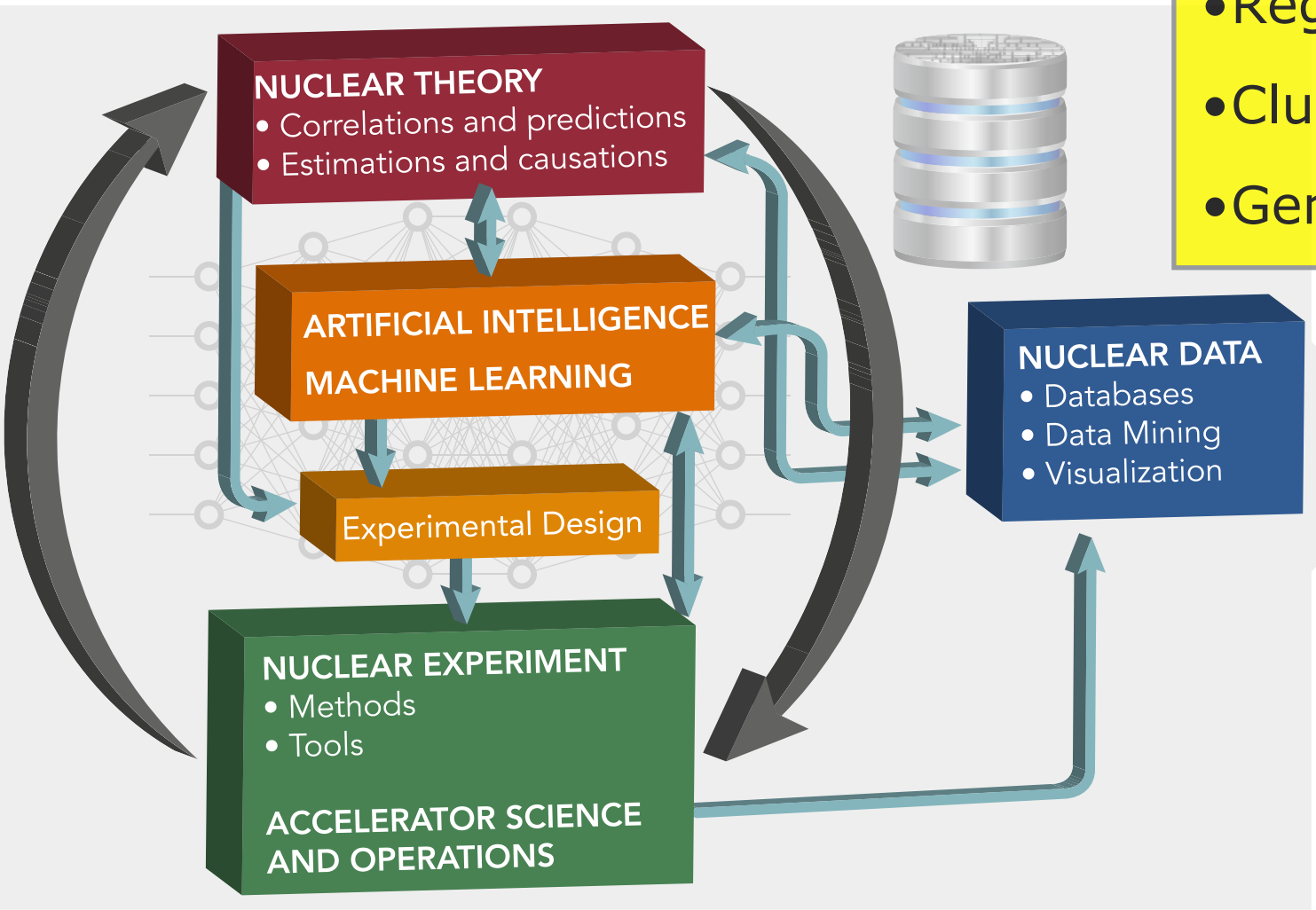
- Classification
- Regression
- Clustering
- Generation



DISCOVERY

APPLICATIONS

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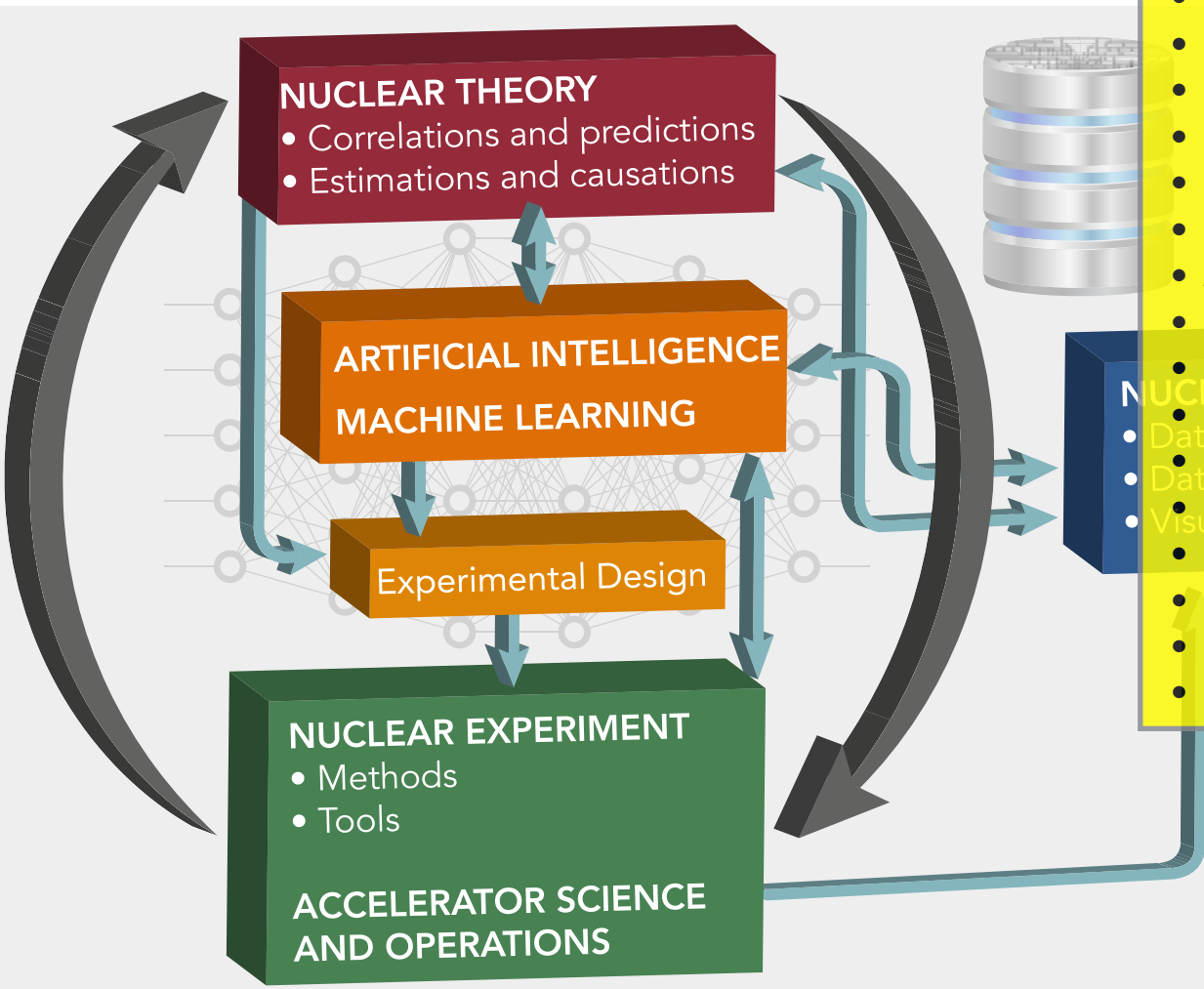
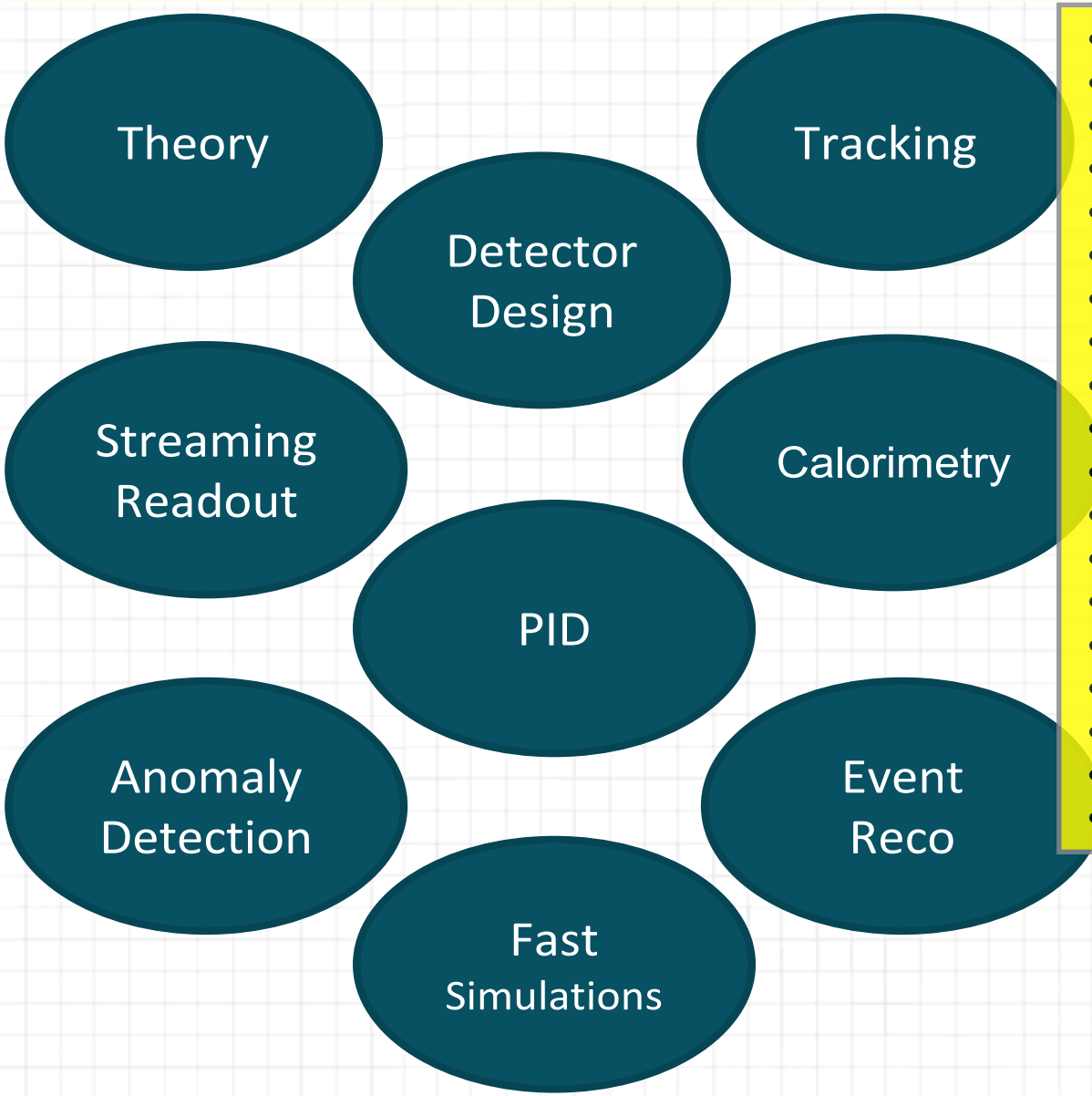


- (Variational) Auto Encoders
- Artificial Neural Networks
- Bayesian Model Averaging/Mixing
- Bayesian Optimisation
- Bayesian Neural Networks
- Convolutional Neural Networks
- Ensemble Methods & Boosting
- Generative Adversarial Networks
- Gaussian Processes
- *k*-Nearest Neighbours
- Kernel Regression
- Logistic Regression
- Long Short-Term Memory
- Principal Component Analysis
- Linear Regression
- Reinforcement Learning
- Recurrent Neural Networks
- Support Vector Machines
- ...

Role of ML and AI in nuclear physics



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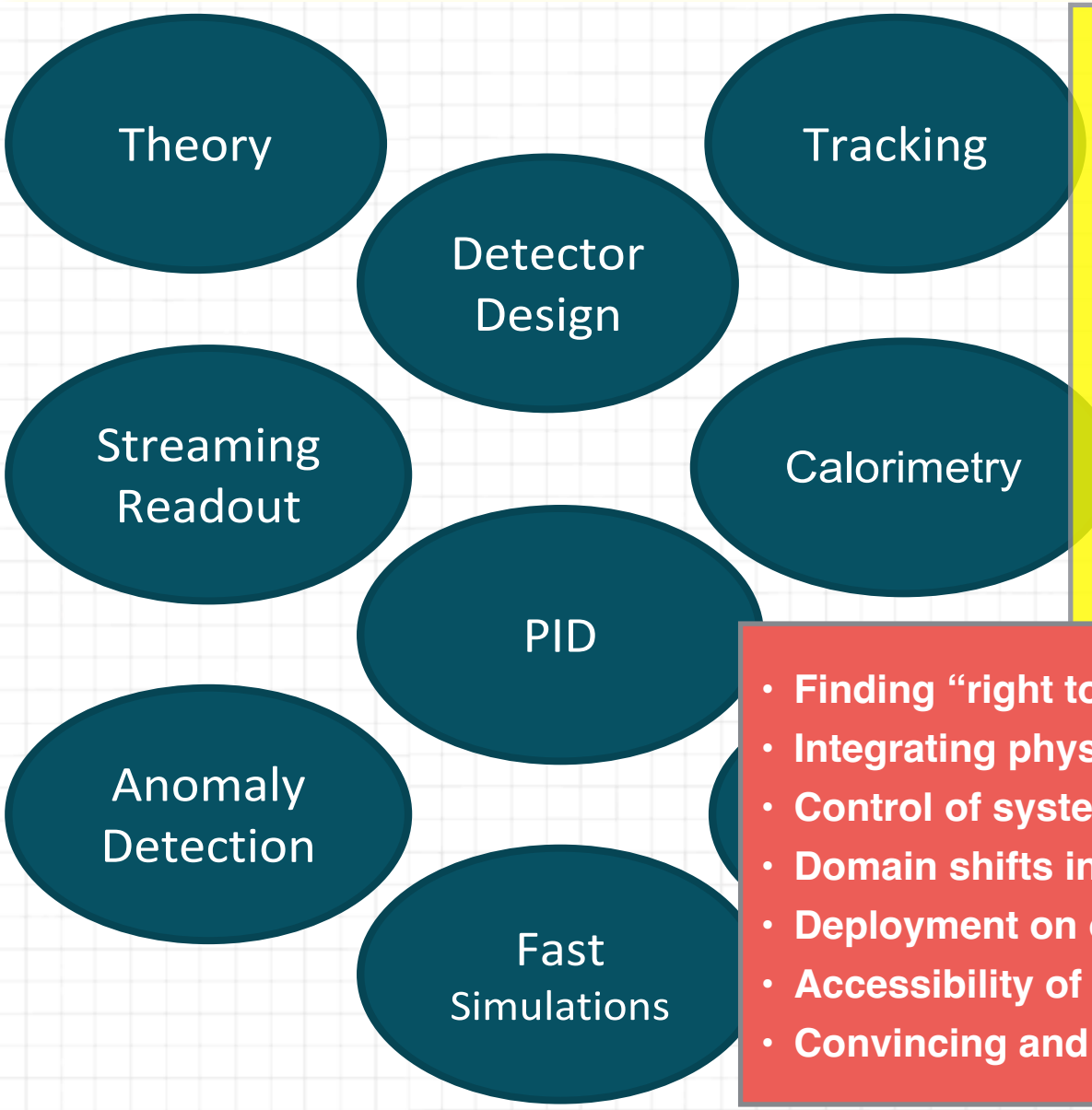
Role of ML and AI in nuclear physics



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- Logistic Regression
- Long Short-Term Memory
- Principal Component Analysis

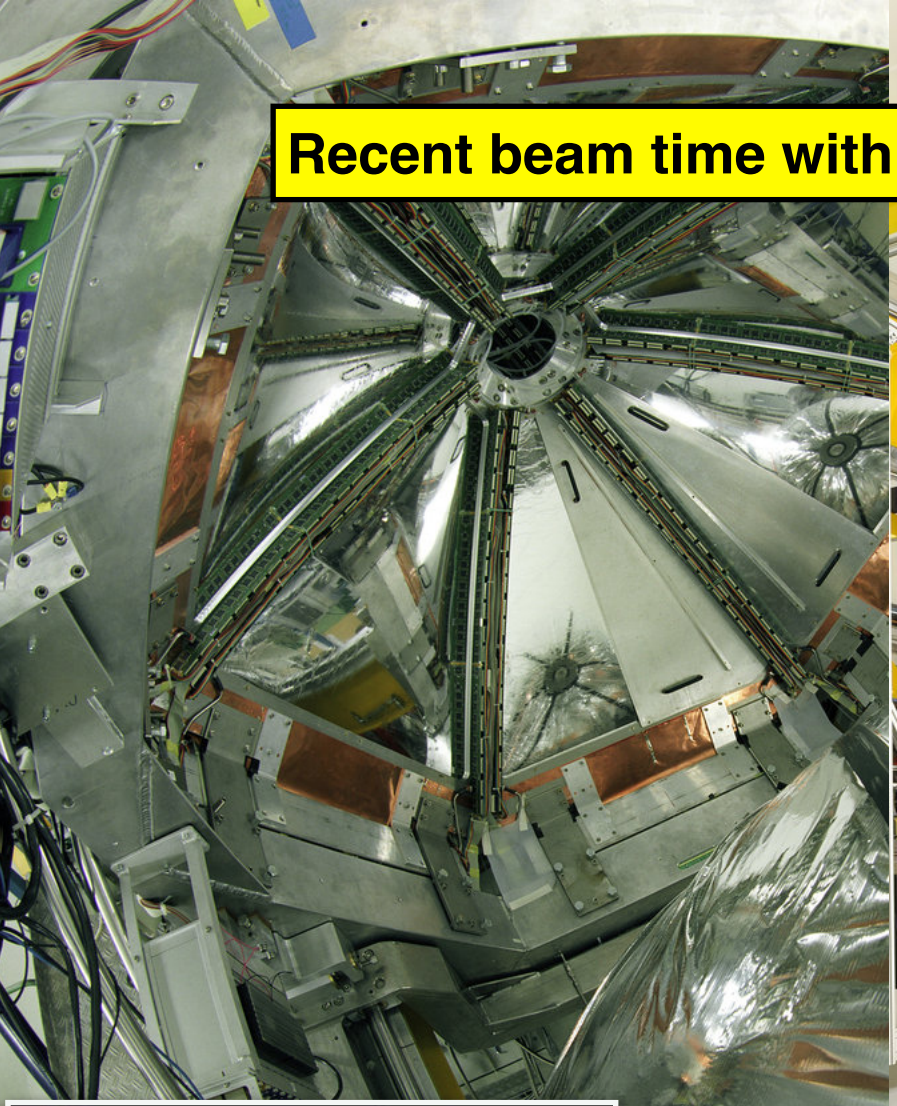
Challenges!

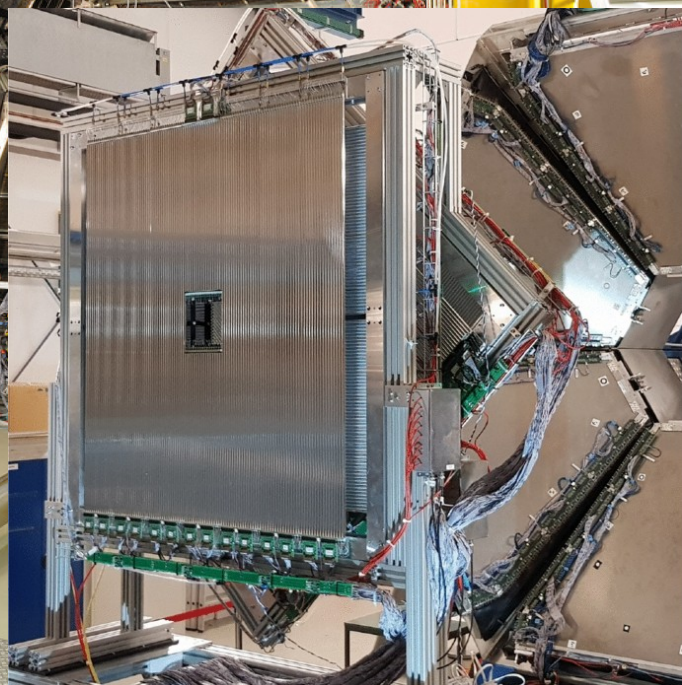
- **Finding "right tool for the right job"!**
- **Integrating physics knowledge.**
- **Control of systematic errors.**
- **Domain shifts in supervised learning.**
- **Deployment on online/embedded architectures.**
- **Accessibility of model/trained data.**
- **Convincing and involving community.**


We have a dream!
(…or a conceptual challenge)

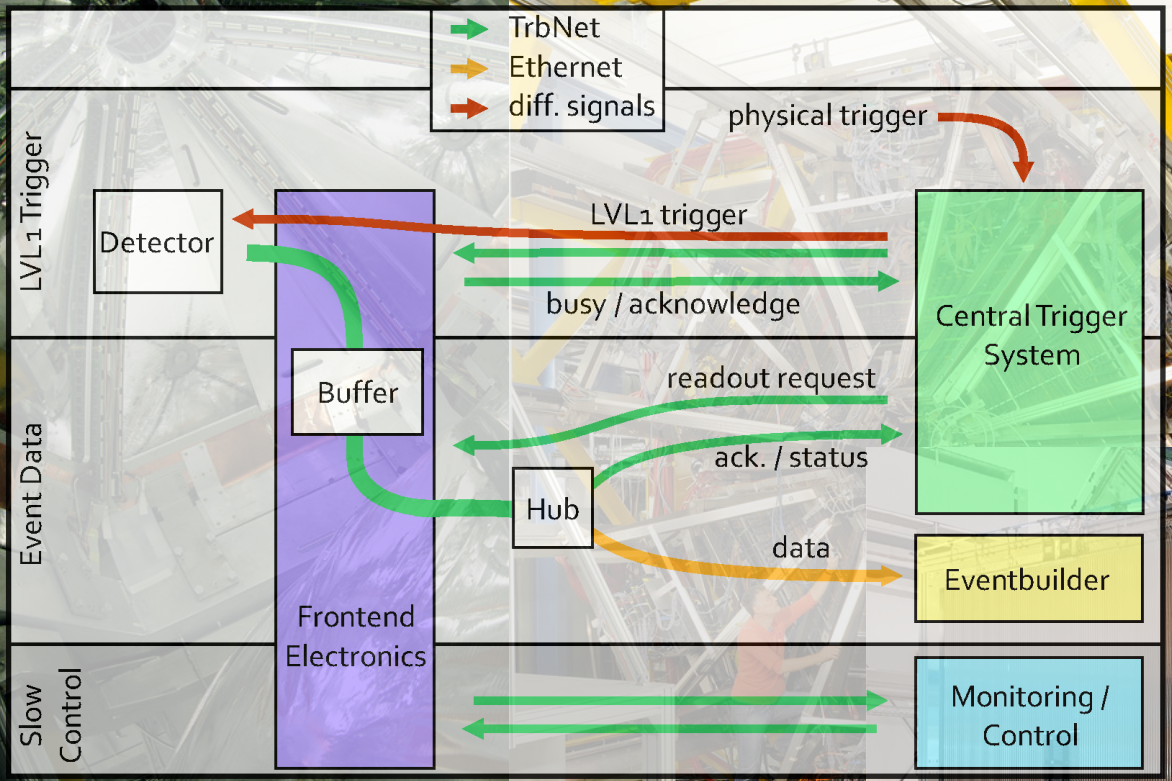

We have a dream!
(…or a conceptual challenge)
Three Waves of AI
DESCRIBE
Handcrafted Knowledge
CATEGORIZE
Statistical Learning
EXPLAIN
Contextual Adaptation

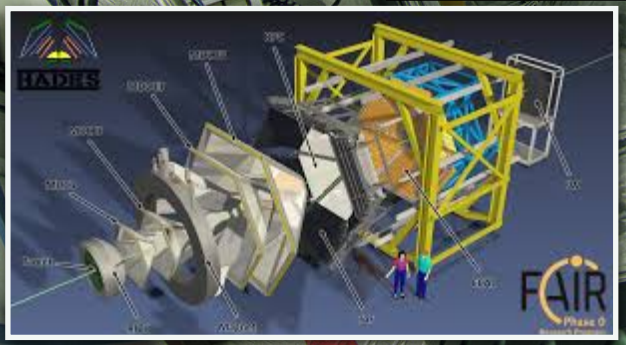
Recent beam time with HADES at FAIR Phase Zero



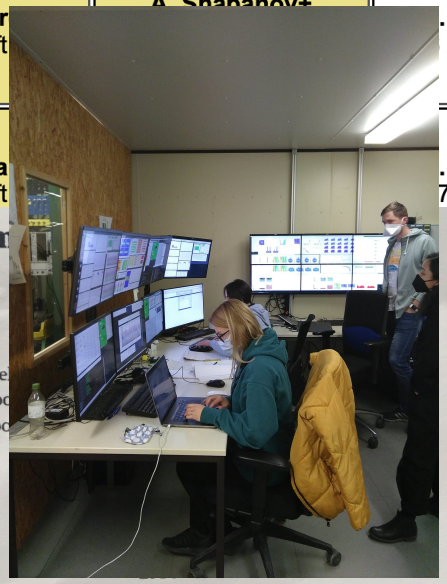


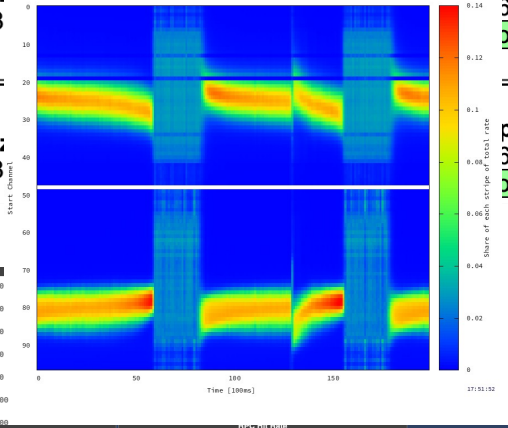
Recent beam time with HADES at FAIR Phase Zero

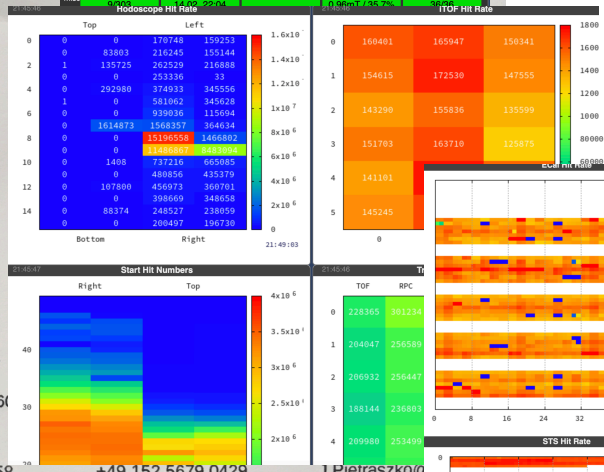


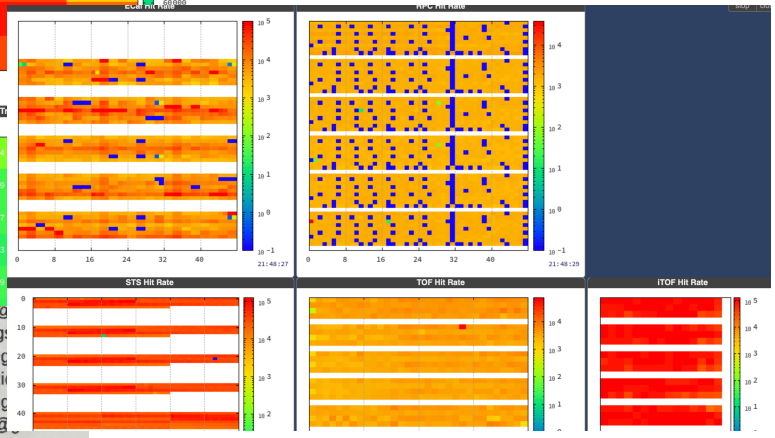


Shift Start	Shift-Leader	DAQ+QA Operator	DAQ-Standby Expert	MDC Operator	RICH Operator	ECAL Operator	Forward STS Operator	Forward RPC Operator	RPC Operator
WEDNESDAY 16-FEB-2022									
16:00	I. Ciepal on shift	A. Shabanov+A.Strach on shift	J. Adamczewski-Musch +49-172-6668324	R. Abou Yassine on shift	J. Friese on shift Info	A. Prozorov +420778028814	K. Sumara on shift +48506334937		L. Lopes +351963609943 Info
THURSDAY 17-FEB-2022									
00:00	J. Rieger on shift	M. Grunwald on shift	M. Traxle +49-6159-7 1348			A. Prozorov +420778028814	J. Rieger on shift +46793046820		L. Lopes +351963609943 Info
08:00	A. Prozor on shift	A. Shabanov+	. Miche 240 11			A. Prozorov +420778	K. Pysz		L. Lopes 509943
16:00	I. Ciepa on shift		. Miche 762401			A. Proz +420778			pes 509943









GSI Telefonnum

Name		private		
HKR SIS				
Strahlenschutz				
Hades cave				
Hades Detector Room "Ede				
Hades Lower Counting Roo				
Hades Upper Counting Roo				
Hades Cave Entrance				
NE5 Entrance				
Cryo				
Network				
FRS				
guest house GSI				
Christian Müntz	2153	069-494461		
Christian Wendisch	2720			
Erwin Schwab	2448	06103-571536		
Gosia Gumberidze	1825			
Jan Michel	2449 / 069-798-47081			
Jerzy Pietraszko	1632	06150-5509158	+49 152 5679 0429	J.Pietraszko@
Joachim Stroth	2151 / 069-798-47083	0170-9604445	0174-328-1534	J.Stroth@gs
Jochen Markert	2885	06074-4074235		j.kempter@g
Jörn Adamczewski-Musch	1337		0172-6668324	j.adamczewski
Michael Traxler	1348	06221-7500157	0174-3281572	M.Traxler@g
Peter Zumbruch	1435		0173-6568626	P.Zumbruch@
Torsten Heinz	2781	06162-982292	0175-3884066	T.Heinz@gsi.de
Vladimir Pechenov	1649		0176-99014501	V.Pechenov@gsi.de

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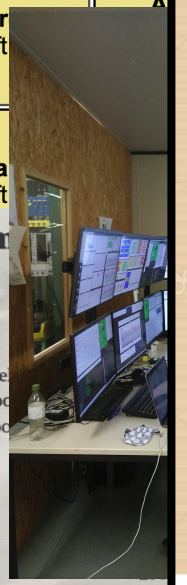
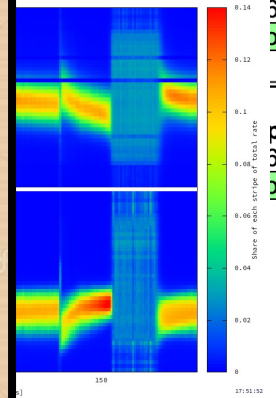
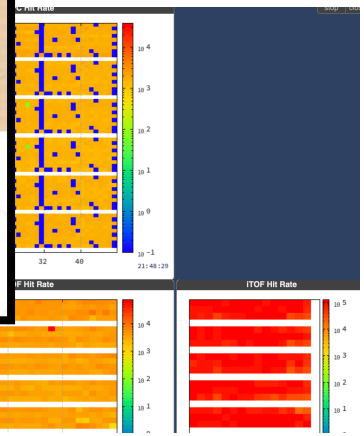




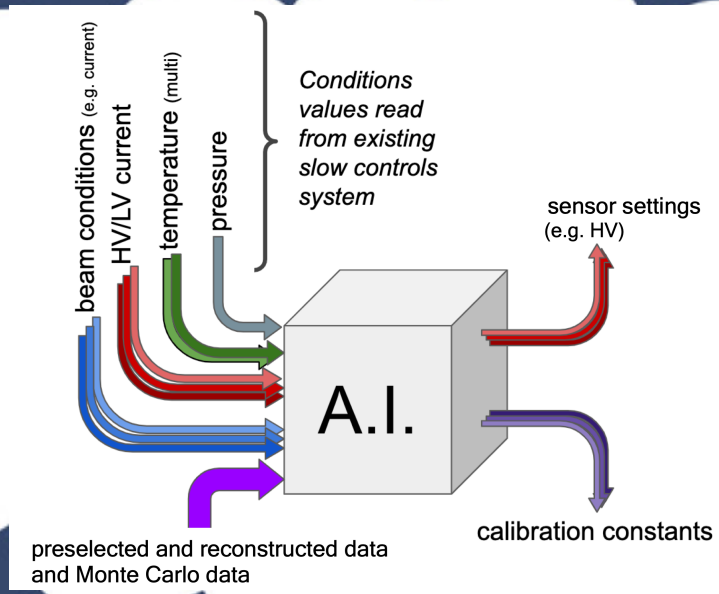


GSI Telefonnum

Name	
HKR SIS	
Strahlenschutz	
Hades cave	
Hades Detector Room "Ede	
Hades Lower Counting Roo	
Hades Upper Counting Roo	
Hades Cave Entrance	
NE5 Entrance	
Cryo	
Network	
FRS	
guest house GSI	

Christian Müntz	2449			
Christian Wendisch				
Erwin Schwab				
Gosia Gumberidze				
Jan Michel				
Jerzy Pietraszko				
Joachim Stroth	2151 / 069-798-47083	0170-9604445	0174-328-1534	J.Stroth@gs
Jochen Markert	2885	06074-4074235		j.kempter@g
Jörn Adamczewski-Musch	1337		0172-6668324	j.adamczewski
Michael Traxler	1348	06221-7500157	0174-3281572	M.Traxler@g
Peter Zumbruch	1435		0173-6568626	P.Zumbruch@
Torsten Heinz	2781	06162-982292	0175-3884066	T.Heinz@gsi.de
Vladimir Pechenov	1649		0176-99014501	V.Pechenov@gsi.de


beam conditions (e.g. current)
HV/LV current
temperature (multi)
pressure
Conditions values read from existing slow controls system
sensor settings (e.g. HV)
A.I.
calibration constants
preselected and reconstructed data and Monte Carlo data



Why?

- Beams at high intensities, harsh environment, increasing #sensors + holistic
- In-situ event reconstruction will rely on quality beam & calibrated sensors
- High operational costs, limited beam time, and human resources
- Remote control has become more important (pandemic)

Towards an International Network

For Multiphysics Modelling, Machine learning and Model-based Control in Accelerator Sciences and Technologies

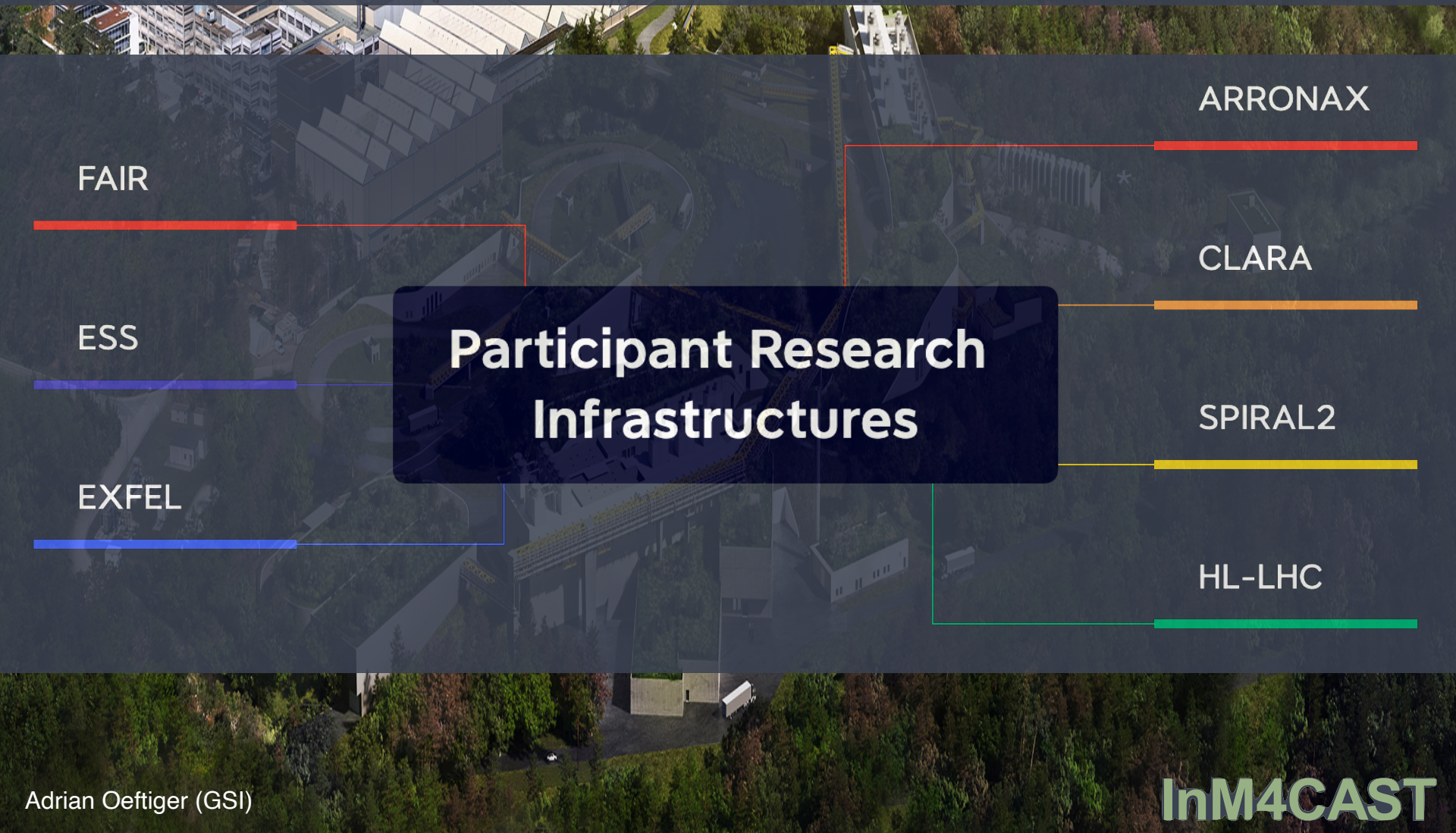
Bringing together experts in accelerators and artificial intelligence to tackle challenges of present and future research infrastructures

Adrian Oeftiger (GSI)

InM4CAST

Towards an International Network

For Multiphysics Modelling, Machine learning and Model-based Control in Accelerator Sciences and Technologies



Adrian Oeftiger (GSI)

InM4CAST

Towards an International Network

For Multiphysics Modelling*, Machine learning and Model-based Control in Accelerator Sciences and Technologies

Parameter space scans
Fast and reliable
Data generation for models building

Smarter simulations

Detecting
Classifying
Preventing

Anomalies

HORIZON2024-INFRATEC-01-01*

Fast and reliable tuning
Beam time increase

Operation and control

Teaching, energy, society applications, ...

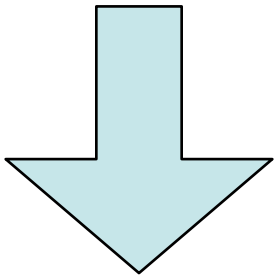
Transverse applications

Adrian Oeftiger (GSI)

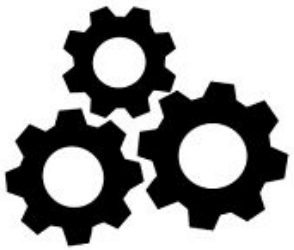
InM4CAST


FAIR

FAIR



Findable **A**ccessible **I**nteroperable **R**eusable

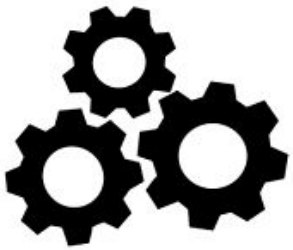


FAIR

- Involved in ESCAPE, PUNCH4NDFI, EuroLabs
- Observer in EOSC

Findable **A**ccessible **I**nteroperable **R**eusable






Challenges in *federated* computing?

The FAIR principles are guidelines for making data more discoverable, accessible, and reusable. The term "federated" in the FAIR context refers to the idea of connecting or integrating data across different sources or repositories to enhance its usefulness and accessibility. It aims to overcome the limitations of centralized data repositories by allowing data to be distributed across multiple sources while maintaining interoperability.

ChatGPT

Challenges in *federated* computing?

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ChatGPT

- **Federation** is in the **genes** of nuclear **physicists** (or researchers in general!)
- "Federated computing" in the context of the "FA**I**R" principle (interoperability)? Do not make it a goal in itself, **keep in mind the objective**.
- Formulate the "**figure-of-merit**", e.g. what are we optimising precisely, what is "useful" and for whom? What is the price tag (financial sustainability?).
- Do not limit yourself to the European context: **researchers are working internationally** (shouldn't it be open science?).
- It will only work if the research community sees the value of "federated computing". **Put the researcher and its research objectives central**!

Challenges in (federated) computing in NP
- five concluding propositions

- Computing in NP is **challenged** by the **complexity** in its future data processing, operation, and handling, preserving precision in a **large "dynamic range"**.
- The **large diversity and standards** within NP communities adds another degree of **complexity**.
- **ML/AI has an enormous potential** on various computational fronts. **ML/AI** as a "game changer" in data processing and **experiment operation**.
- The basis of successful **federative computing** is commonly **agreed** (interface) **standards**.
- **Federated computing** valuable if the **research** interest is **central** within an **international focus**.

Johan Messchendorp (GSI/FAIR)
j.messchendorp@gsi.de