



FAIR (computing) goes F.A.I.R.

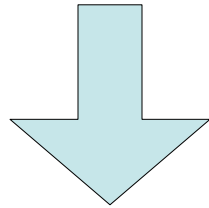




FAIR

The logo features the word "FAIR" in a bold, black, sans-serif font. A stylized orange arc, resembling a partial circle or a path, curves around the letters "A" and "I". At the top of this arc is a solid orange circle, which serves as the dot for the letter "i".

FAIR



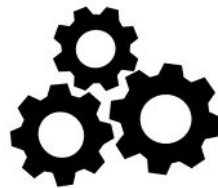
F
Findable



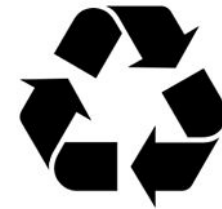
A
Accessible



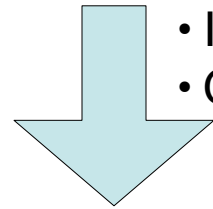
I
Interoperable



R
Reusable



FAIR



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

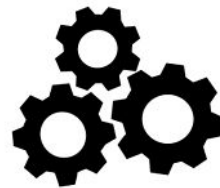
F
indable



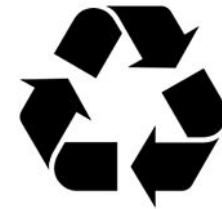
A
ccessible



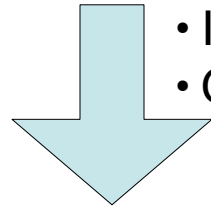
I
nteroperable



R
eusable



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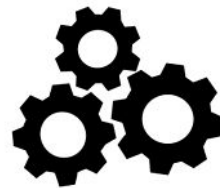
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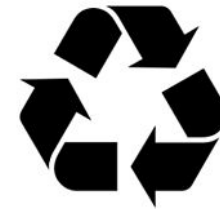
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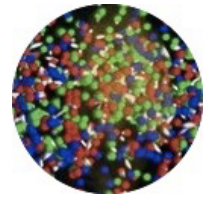
R
eusable



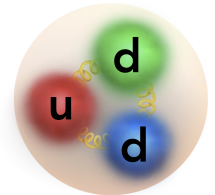
Why? How? What? Who?

Computing at FAIR

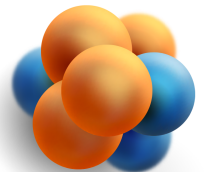
Some key characteristics to take note of!



Hot and Dense
Nuclear Matter



Hadrons



Atomic Nucleus



Nuclei in the Cosmos

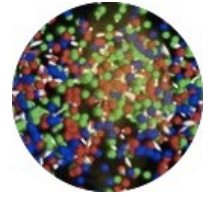
u up	c charm	t top	γ photon	H Higgs boson
d down	s strange	b bottom	g gluon	
ν_e electron neutrino	ν_μ muon neutrino	ν_τ tauon neutrino	Z^0 Z boson	
e electron	μ muon	τ tau	W^\pm W boson	Charge bosons

Fundamental Interactions

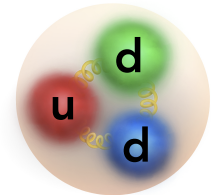
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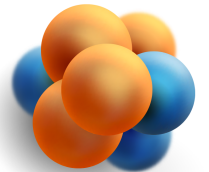
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Hot and Dense
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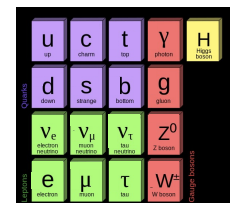
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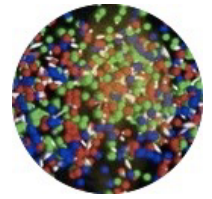


Fundamental Interactions

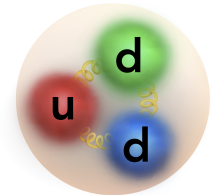
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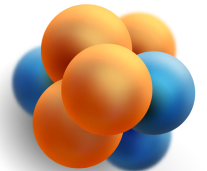
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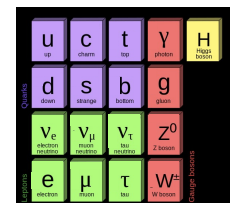
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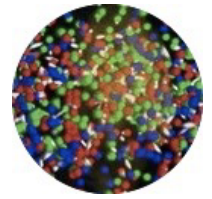


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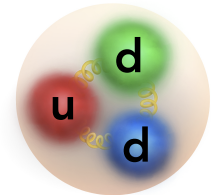
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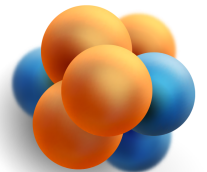
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- **New developments** in hard- (GPU, ARM, QC,...), software (ML/AI), in data processing (triggerless readouts) and management (F.A.I.R., federated infrastructures).



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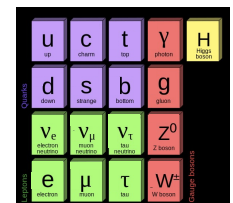
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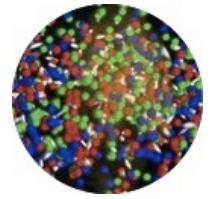


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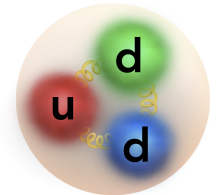
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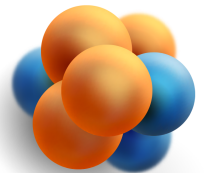
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- Computing support **centrally organised** & understaffed compared to HEP communities!



Hot and Dense Nuclear Matter



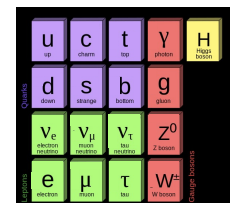
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Nuclei in the Cosmos



Fundamental Interactions

FAIR and open science - why?

What to gain (or to lose)?



FAIR and open science - why?

What to gain (or to lose)?

- The **sticks**: funding, evaluation criteria, moral obligation, ...



FAIR and open science - why?

What to gain (or to lose)?

- The **sticks**: funding, evaluation criteria, moral obligation, ...

- The **carrots**:

- *Ease* the accessibility and exchange of resources & results.
- *Long-term preservation* of data/software/services.
- Enhance *quality* of research.
- Enrich *scientific output*.
- Enhance synergy with other disciplines.
- Enable "citizen science".

+

Importance

-



FAIR and open science - why?

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Importance

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- *Long-term preservation* of data/software/services.

- Enhance *quality* of research.

- Enrich *scientific output*.

- Enhance synergy with other disciplines.

- Enable "citizen science".



- The **advice**: invest "there were it makes sense". **NO free lunch.**

FAIR and open science - how?

Formulate *conceptual* design report for FAIR computing

Conceptual Design Report for FAIR Computing

Mohammad Al-Turany, Volker Friese, Thorsten Kollegger,
Bastian Loehner, Jochen Markert, Johan Messchendorp,

Andrew Mistry, Thomas Neff, Adrian Oeftiger, Michael Papenbrock,
Stephane Pietri, Shahab Sanjari, Tobias Stockmanns

October 2, 2023

Abstract

This Conceptual Design Report (CDR) presents the plans of the computing infrastructure for research at FAIR, Darmstadt, Germany. It presents the computing requirements of the various research groups, the policies for the computing and storage infrastructure, the foreseen FAIR computing model including the open data, software and services policies and architecture for the periods starting in 2028 with the "first science (plus)" phase to the modularized start version of FAIR. The overall ambition is to create a federated and centrally-orchestrated infrastructure serving the large diversity of the research lines present with sufficient scalability and flexibility to cope with future data challenges that will be present at FAIR.

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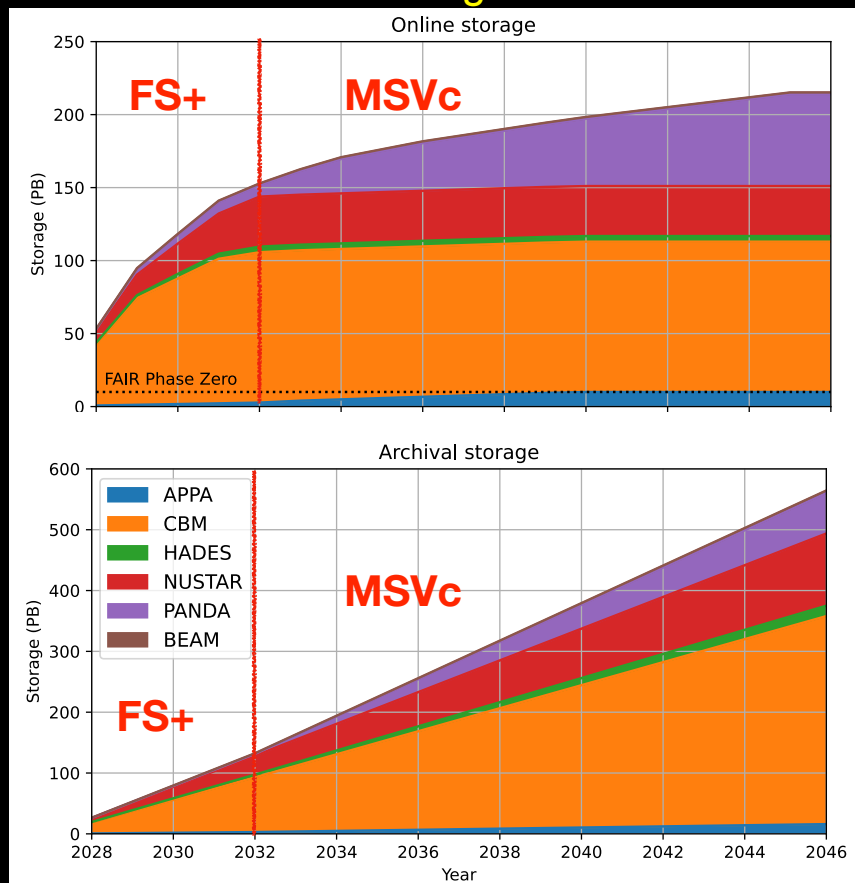
FAIR Computing “CDR”?

...mostly about estimating required resources...

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Storage

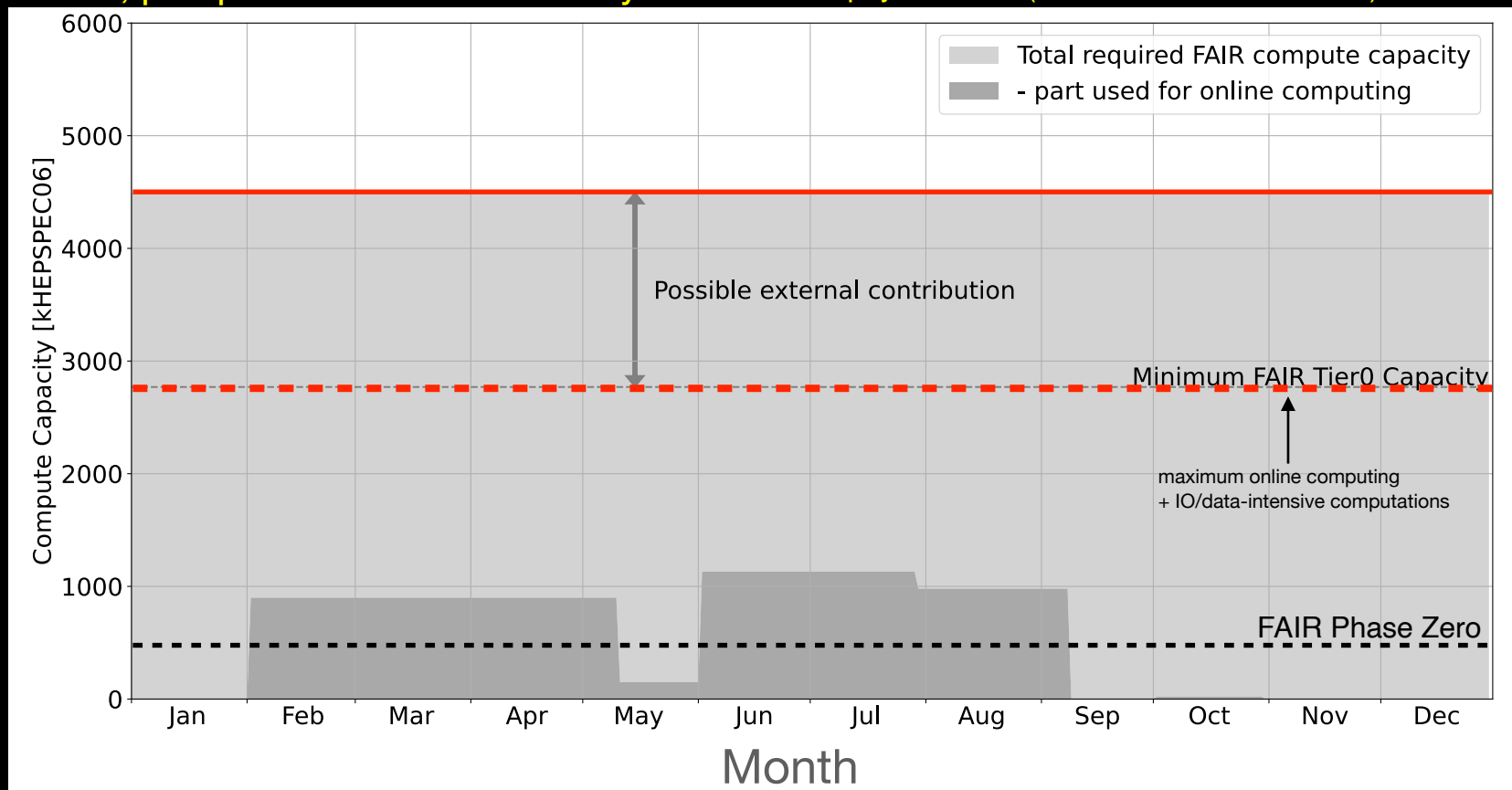


FAIR Computing “CDR”?

...and defining the necessary compute capacities...

MSVc, perspectives for a “nominal year”

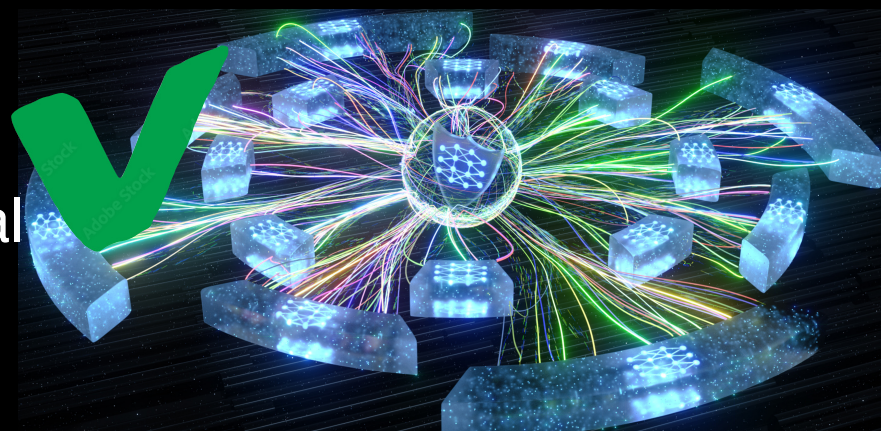
1 physical core (Intel E5-2680v4@2.4GHz) ~22 HEPSPEC06



FAIR and distributed computing?

...main buzzword: “federated computing” ...

- **Federation**: the act of uniting smaller or more localised entities to create a larger entity for mutual benefit, with agreed mixture of common policies and local autonomy.
- **Consolidation**: the act of reducing the number of entities by dissolution of existing ones and creation of a single larger entity.



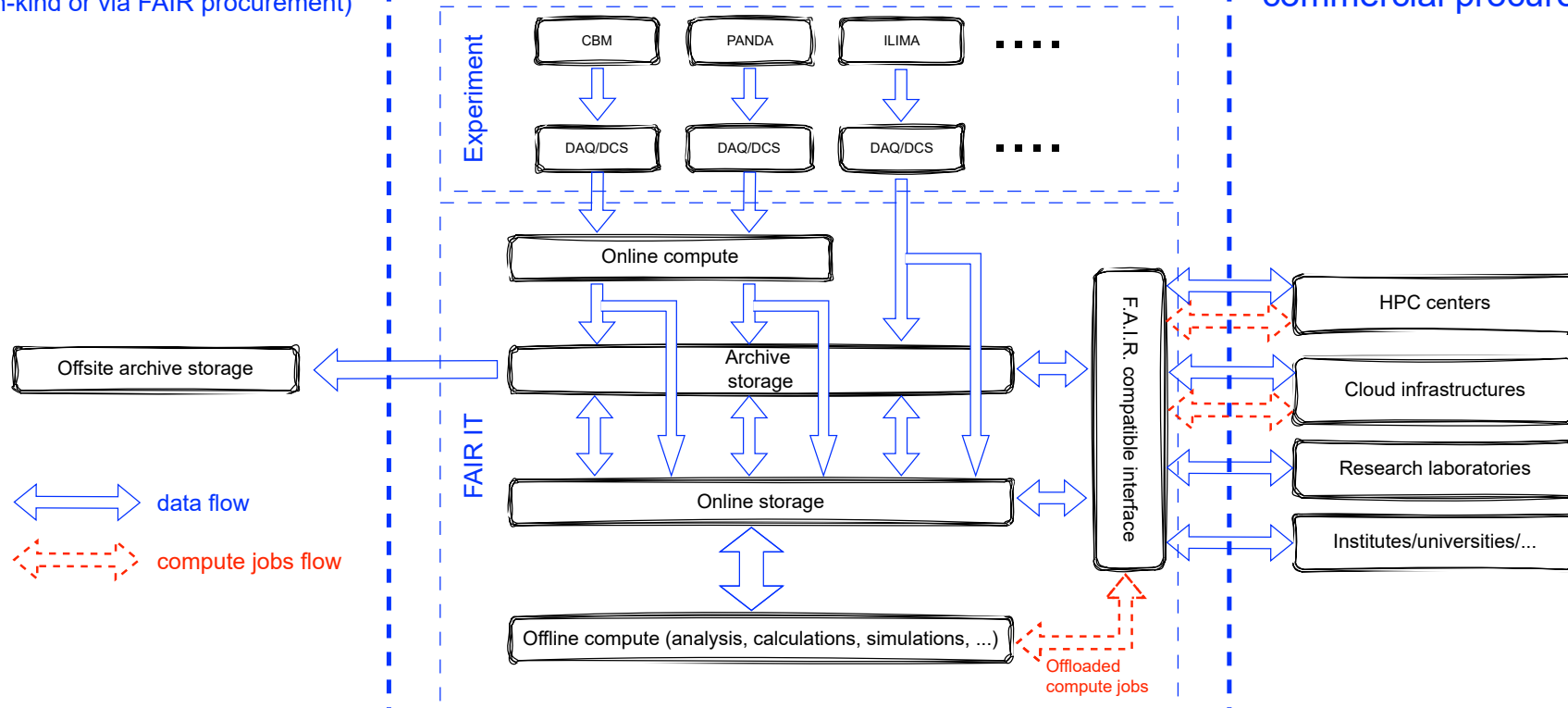
Computing model

...with a central role of F.A.I.R. ...

FAIR member states
(in-kind or via FAIR procurement)

FAIR on campus

Academic collaborations or
commercial procurements



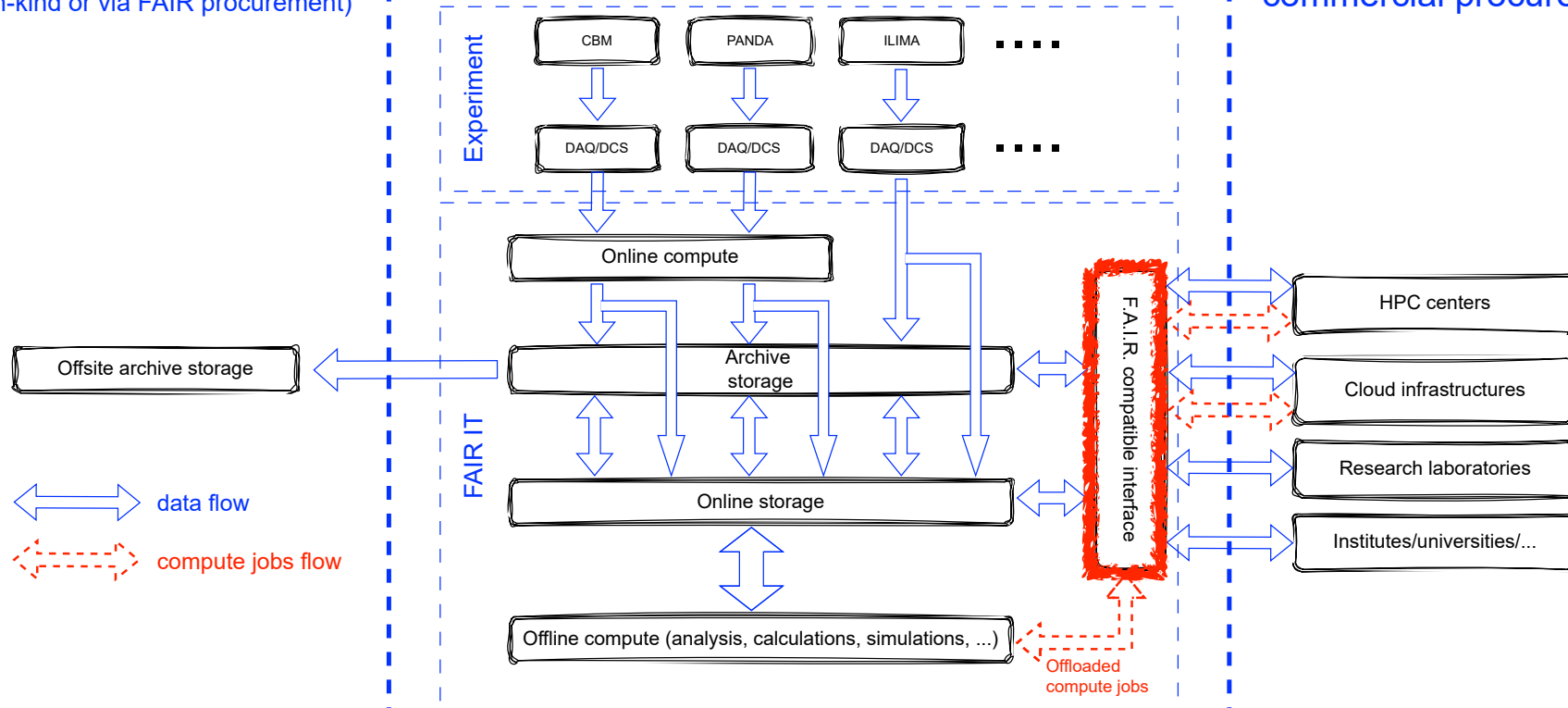
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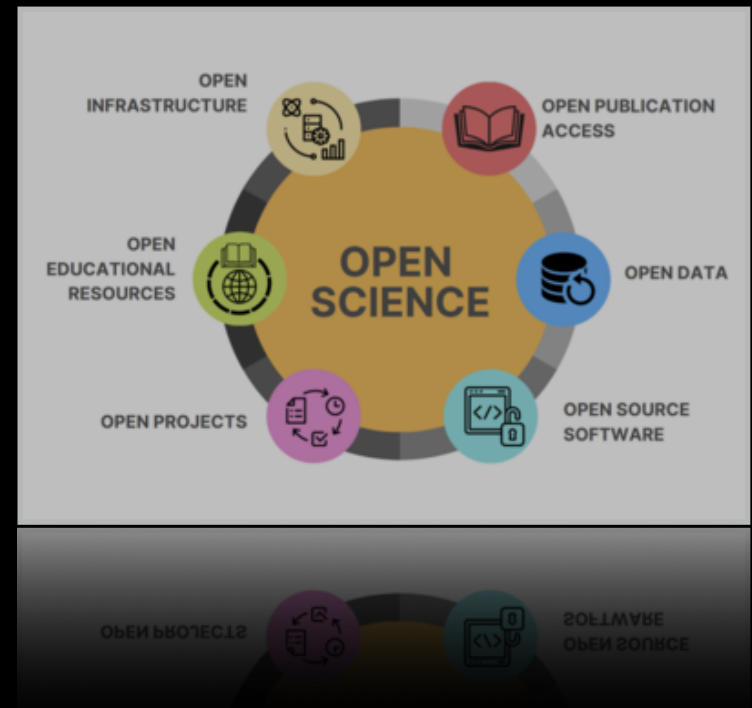
Academic collaborations or
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FAIR goes F.A.I.R.?

...bit more than just conceptual box on a diagram?

- **Align** with open-science policies setup for **GSI**!
- FAIR-**IT** provides F.A.I.R.-*supportive* base infrastructure
- **Research lines** are *responsible* for the “openness” of their data & software!



Principles	Policies & Services
Findable F	?
Accessible A	?
Interoperable I	?
Reusable R	?

Principles	Policies & Services
Findable F	?
Accessible A	<ul style="list-style-type: none"> • Data and software produced and dedicated for FAIR communities and publications centrally stored. • Data will be accessible using standard http protocols, possibly with XRootD on the frontend and Lustre at the backend. • AAI will be token-based and integrated with eduGAIN in line with ongoing concepts introduced within ESCAPE/EOSC. • Data and software available under a suitable open licence (such as GPL or CC BY).
Interoperable I	?
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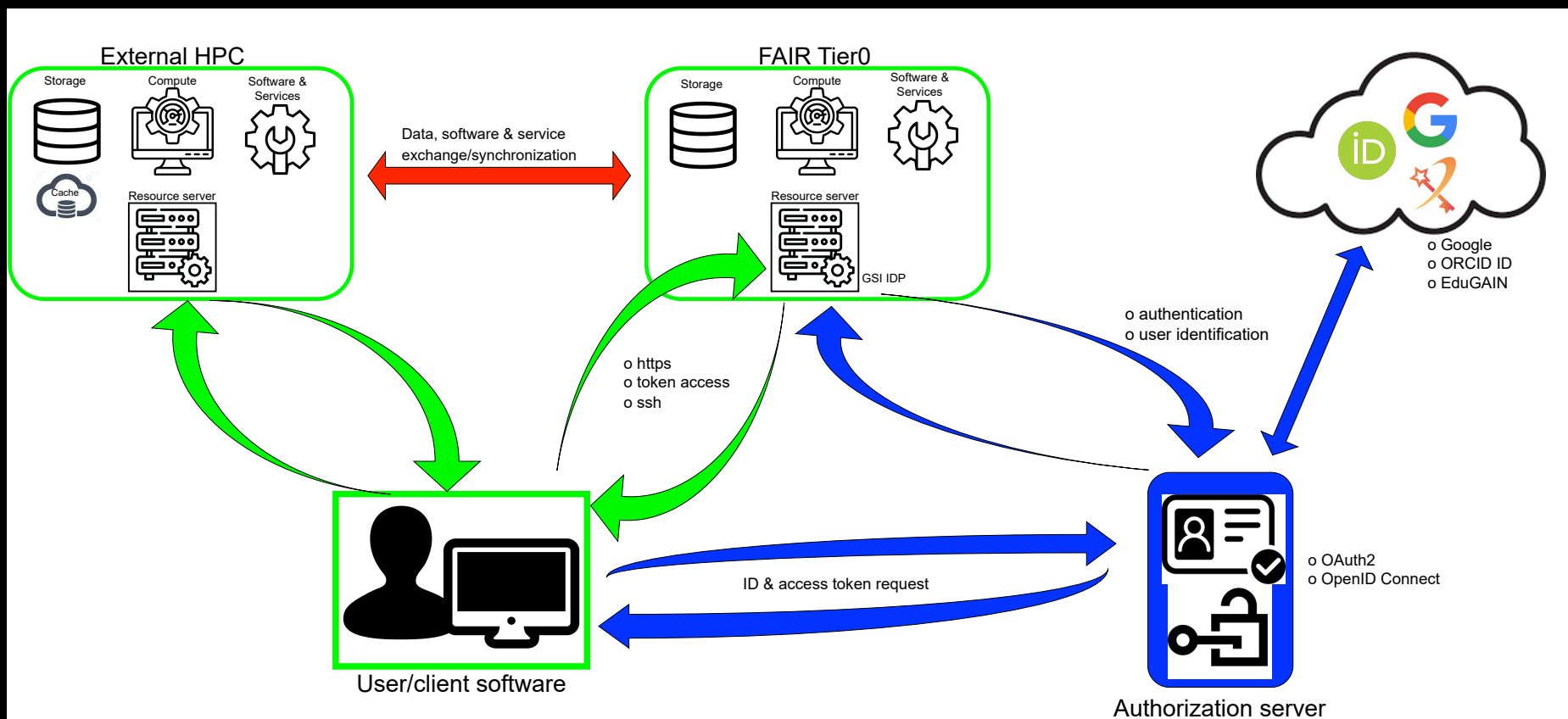
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Findable F	<ul style="list-style-type: none"> • Centrally orchestrated storage and access of data. • Consistent usage of Persistent IDentifiers (PID) such as Digital Object Identifiers (DOI) for data and metadata. • Expand the GATE environment available at GSI. • Promote and support the open-source scientific software and service repository (OSSR) within the ESCAPE collaboration.
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Interoperable I	<ul style="list-style-type: none"> • Participate in community-wide open-science initiatives, projects & programs on institutional, national, and European levels. • Follow-up the “Datalake” concept developed within ESCAPE. • Support the OSSR service (see above) to encourage the use of common software and services within the research domain. • Use common AAI services together with partner institutes and facilities (see above). • Agree upon controlled metadata vocabularies within the research domain of interest.
Reusable R	<p style="text-align: center;">?</p>

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Reusable R	<ul style="list-style-type: none"> • Ensure a successful implementation of the principles described above (“F.A.I.”), the reusability will follow naturally.

FAIR goes F.A.I.R.?

...in a cartoon representation



Web of F.A.I.R. (& FAIR) data and services

...realistic or fiction?



Web of F.A.I.R. (& FAIR) data and services

...realistic or fiction?



EUROPEAN OPEN SCIENCE CLOUD

“Web of FAIR data and services”

WORLD WIDE WEB

INTERNET

NETWORKS

COMPUTERS

Web of F.A.I.R. (& FAIR) data and services

...realistic or fiction?

“Open, trusted, *federation of infrastructures* enabling European researchers to store, share, process, analyse, and reuse digital objects.”

 eosoc

EUROPEAN OPEN SCIENCE CLOUD

“Web of FAIR data and services”

WORLD WIDE WEB

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Web of F.A.I.R. (& FAIR) data and services

...the “black mirror” side of the EOSC dream



Web of F.A.I.R. (& FAIR) data and services

...the “black mirror” side of the EOSC dream

- It is a **great vision!** But still very far away from realising...



Web of F.A.I.R. (& FAIR) data and services

...the “black mirror” side of the EOSC dream

- It is a **great vision!** But still very far away from realising...
- **Digital objects very divers** (size, complexity, policies) among research disciplines: common standards needed.



Web of F.A.I.R. (& FAIR) data and services

...the “black mirror” side of the EOSC dream

- It is a **great vision!** But still very far away from realising...
- **Digital objects very divers** (size, complexity, policies) among research disciplines: common standards needed.
- Very much **focused** towards the **European level**: what about international playfield (like at FAIR)?



Web of F.A.I.R. (& FAIR) data and services

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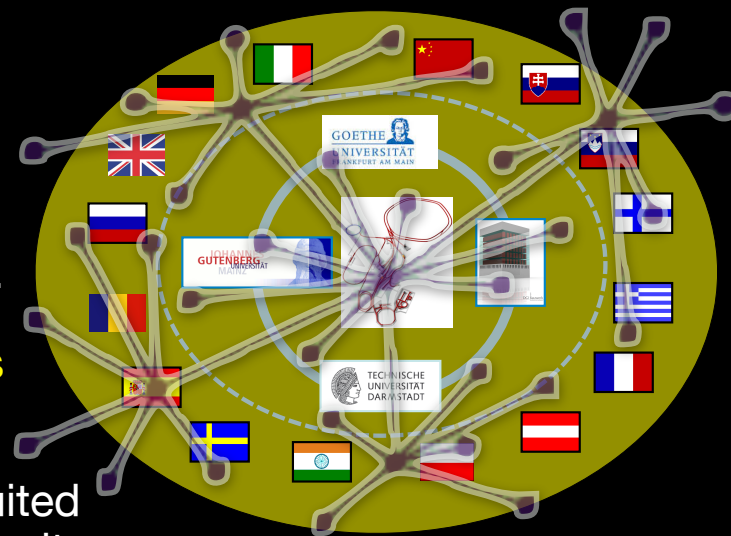
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- Role of **Artificial Intelligence**? Ethical aspects?

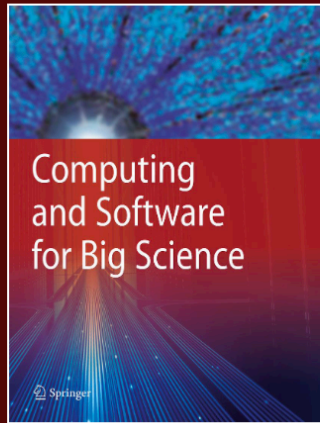


FAIR goes F.A.I.R. in a *nutshell*

- *Grid-like distributed* computing is *dead*, long-live **federated** computing among large centers.
- Effective **resource sharing** at FAIR TIER-0 center, accounting for most of the data-driven computations.
- Federated storage and computing with '**local**' centers using Teralink network & commonly used standards.
- '**Centralised**' data/software management → most suited to incorporate F.A.I.R. principle for our diverse community, introduce and to minimise the operational overhead.
- **Containerised approaches** and other virtualisation methods for flexible compute operations serving diverse community & optimise usage.
- **Data access using http**, possibly with xrootd frontend, lustre backend; AAI using widely accepted standards, weblogin, token-based, eduGAIN.



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We are excited to announce that *Computing and Software for Big Science* has now become a fully open access (OA) journal as of January 2023. This means that we are no longer accepting non-OA articles for submission. All new content published in the journal will be published under an open access licence, and freely available to readers worldwide, enabling the widest possible dissemination and reuse.

Backup material

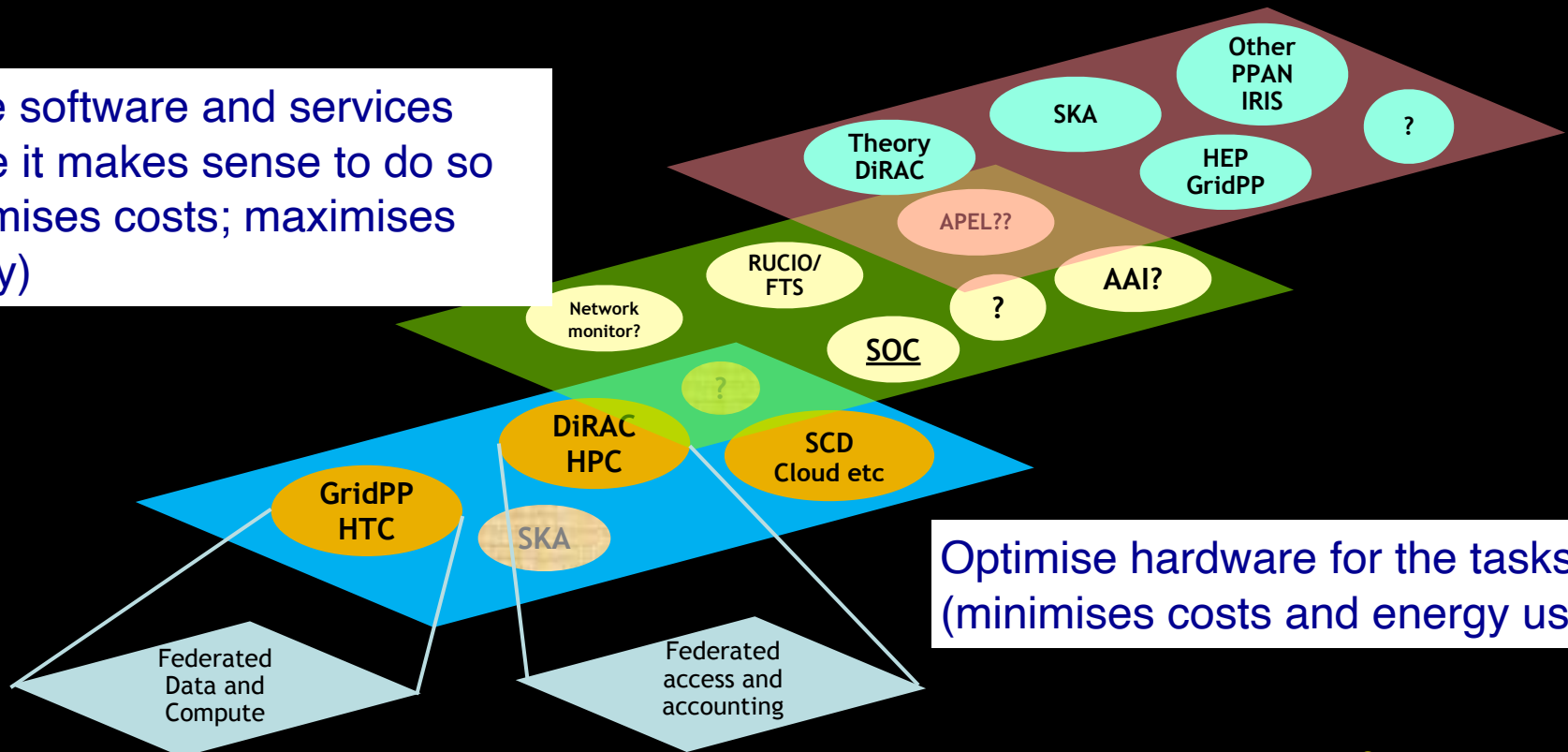
“federated” computing - who ordered that?

- Federation allows composition of new solutions out of existing investment (but you can only rearrange the building blocks if you still have the building blocks).
- Federation enables decision making to be devolved “down” the hierarchy to where it best sits, improving choices and protecting against domination of one community or voice to the detriment of the rest.
- Federation can empower communities in a way that consolidation does not. All these elements become particularly important as the scale grows.
- Federation encourages diversity, of ideas, solutions, and people. It can protect against “group think” and stagnation, and can provide resilience against single points of failure – both geographical and technological.
- Federation enables low risk evaluation and testing of “future” technologies, in particular where they are driven by specific well motivated communities that would otherwise be overlooked or dismissed by a large scale operation with a consolidated approach.
- Federation allows smaller operations to benefit from the full scale of the federation. E.g., security, identity management, accounting and allocation; but also in the building of larger communities to share ideas and solutions.
- Federation allows leveraging of local resources that otherwise would not be available.

“federated” computing - who ordered that?

Recognise that communities need gateway projects that worry about the (evolving) complexity for them.

Share software and services where it makes sense to do so (minimises costs; maximises quality)



FAIR Computing “CDR”?

...a couple of words on that...

- ... focussed towards **research IT**, hence *not* enterprise IT!
- ... aims towards a coherent **vision** for FAIR computing
- ... **supported** by relevant stakeholders including you!
- ... with a description of **requirements** based on best **estimates**
- ... with commonly defined **criteria**
- ... **FAIR players***: **APPA,CBM,HADES,NUSTAR,PANDA,THEORY,BEAM**
- ... considering **FAIR scenarios**: **FS(+)** and **MSV**
- ... present status: **submitted** to ECE/ECSG for approval

*ALICE uses large fraction of computing resources & strong connections with scientific IT@GSI, but considered as “outside” activity, different funding scheme, etc.

FAIR-IT support vs research lines responsibilities

...sensitive topic, hence very relevant!

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The challenges to consider!

- Diversity in requirements among FAIR research lines.
- Roughly two categories:
 1. CBM/PANDA/partly NUSTAR → large scale experiments, online data processing (HTC), heavy dependence on the HPC farm, etc.
 2. APPA/partly NUSTAR/THEORY → specific “use cases”, smaller scale, very diverse and broad communities, not necessarily requiring HPC, etc.
- Cost efficient operation of computing becoming important.

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FAIR-IT support for research

FAIR-IT support vs research lines responsibilities

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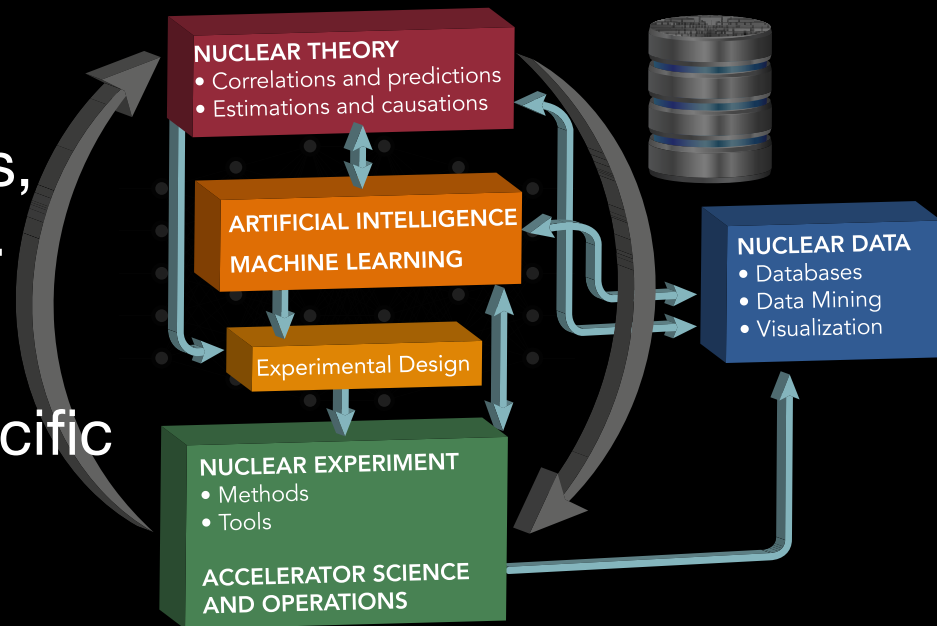
FAIR-IT support for research

- Responsibility: “*at the end of the fibres from the experiment*”.
- Define and setup interfaces between experiment/user and compute/storage.
- Promote as much as reasonably acceptable common interfaces, hard/software infrastructures etc.
- Provide VMs, cloud service to minimise “idle” computers.
- Support commonly-used services/frameworks, e.g. Fairroot, FairMQ, CDash, Gitlab, ...
- Maintain a strong local scientifically-based IT team well integrated within the various experiments with network/interface to experts outside FAIR (f.e. GEANT, ROOT, ...).

R&D aspects to investigate/follow-up

...that potentially reduce costs, provide more physics output...

- Evaluate applications of ML/AI, e.g. smart experiment control and (online) event processing, smart simulations.
- Deployment/benchmarking of algorithms on accelerator cards, ARM, FPGA, QC (long term), ...
- Developments in ESCAPE, PUNCH4NFDI, *i.e.* domain-specific initiatives.



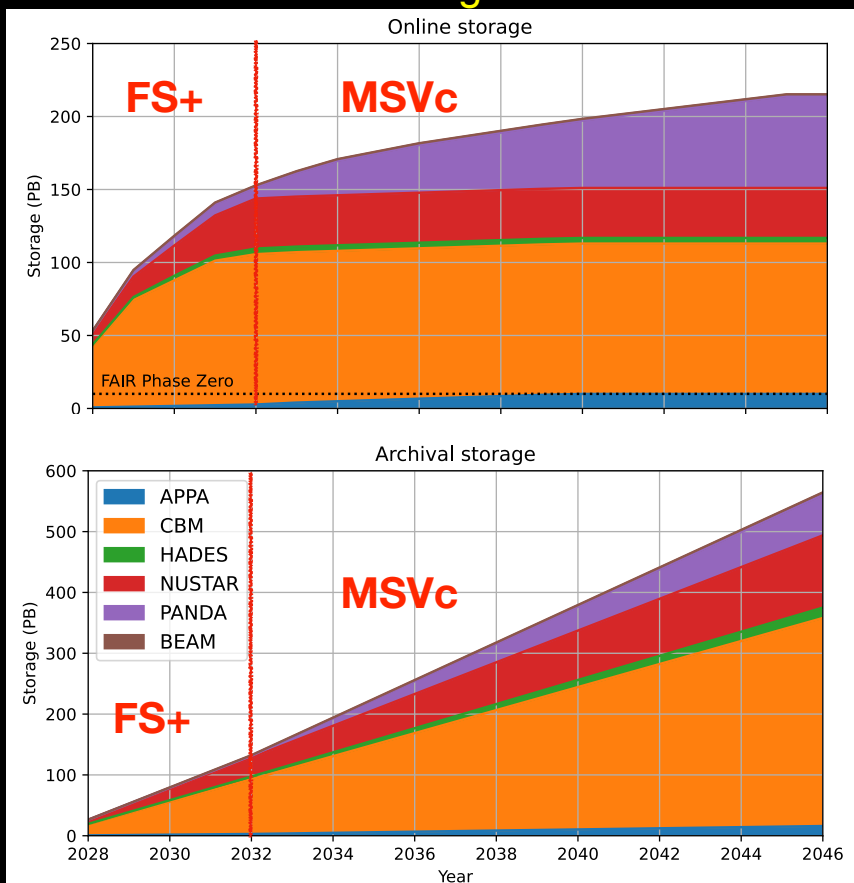
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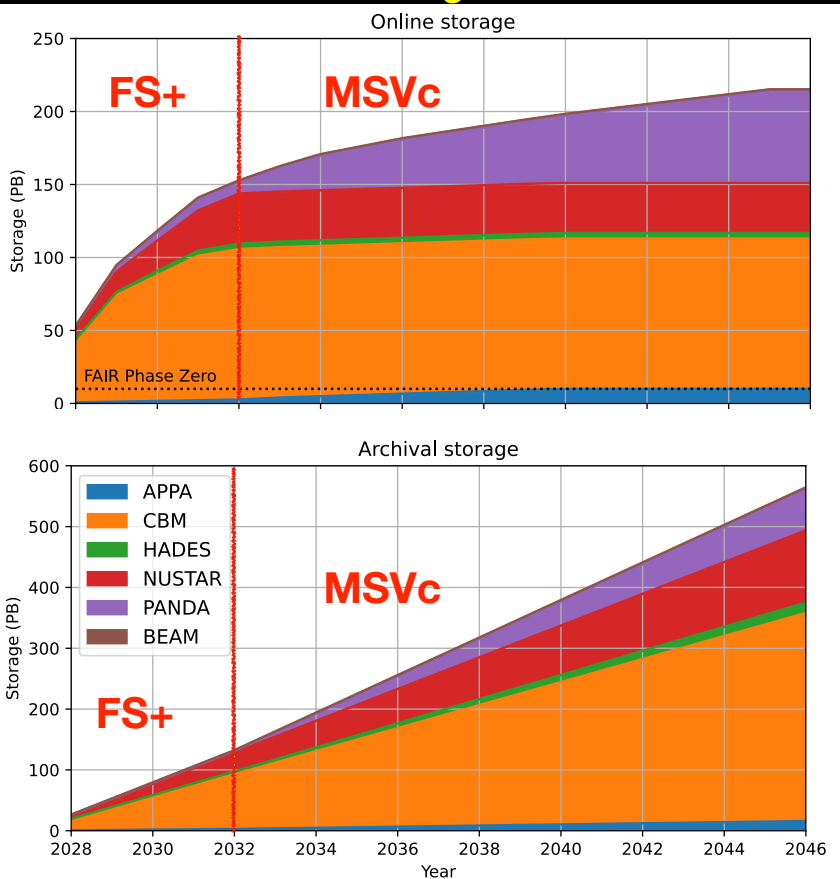
Storage



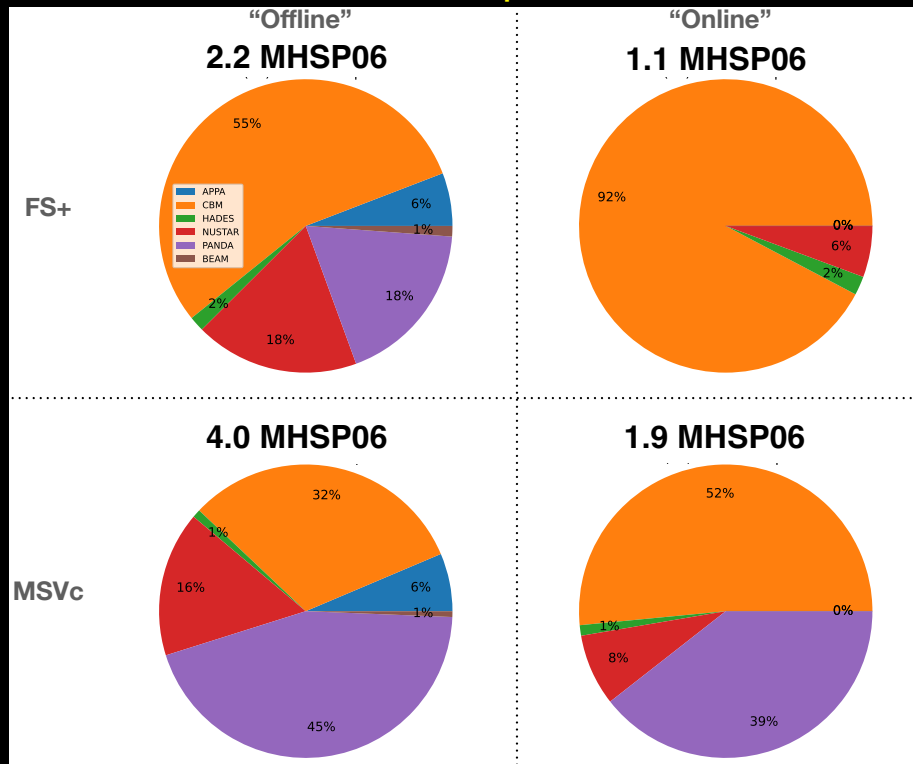
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Storage



Compute



- 1 physical core (Intel E5-2680v4@2.4GHz) ~22 HSP06
- Reference: FAIR Phase Zero ~0.5 MSP06