

Status and Progress of ILDG



Basavaraja BS, P. Fuhrmann, H. Simma

IBERGRID
Benasque

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1. Motivation

2. Basic Concepts of ILDG

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4. Summary and Outlook

Sidetrack

- Usefulness of FAIR data concept
- German funding stream towards FAIR data in the EOSC
- Product: Flexible Meta Data / File Catalogue with strict meta data checking and fine grained Access Control.

QCD on the Lattice

Quantum Chromodynamics (QCD)

Computation of hadronic observables (masses, formfactors, ...) from first principles and beyond perturbation theory:
“path integral”

$$\langle Q \rangle = \int Q(\mathbf{C}) \cdot e^{S(\mathbf{C})} D[\mathbf{C}]$$

Where

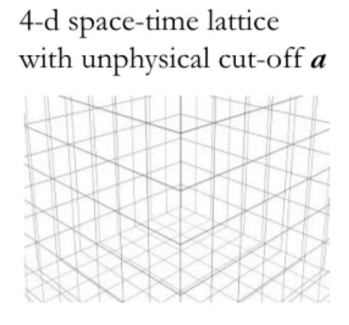
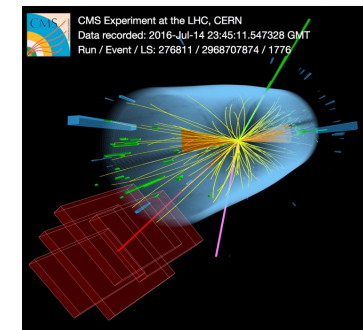
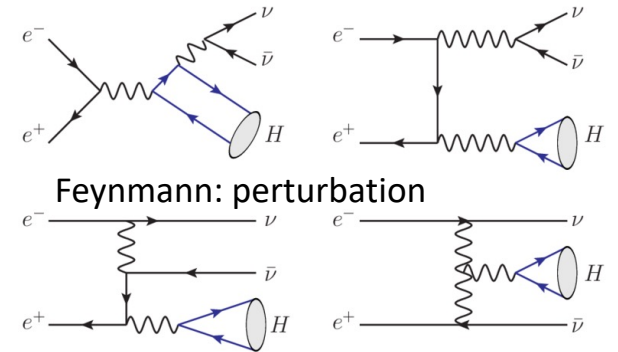
\mathbf{C} = gluon (and quark) field at all points in **4d space time**

S = classical action (\leftrightarrow field equations similar to Maxwell)

Lattice QCD

- discretization: fields defined only on a finite lattice e.g. $V \sim 50^3 \times 200 = 25$ million sites
- integration in **$O(10) \times V$ dimensions**: importance sampling of field configurations $\{C_i\}$ with **weight $e^{-S(C_i)}$** by a Markov Chain Monte-Carlo (MCMC) simulation

$$\langle Q \rangle \approx \frac{1}{N} \sum_{i=1}^N Q(\mathbf{C}_i) \cdot e^{S(\mathbf{C}_i)} \quad (N \rightarrow \infty, \text{ lattice spacing} \rightarrow 0)$$



Lattice QCD Simulation and Data

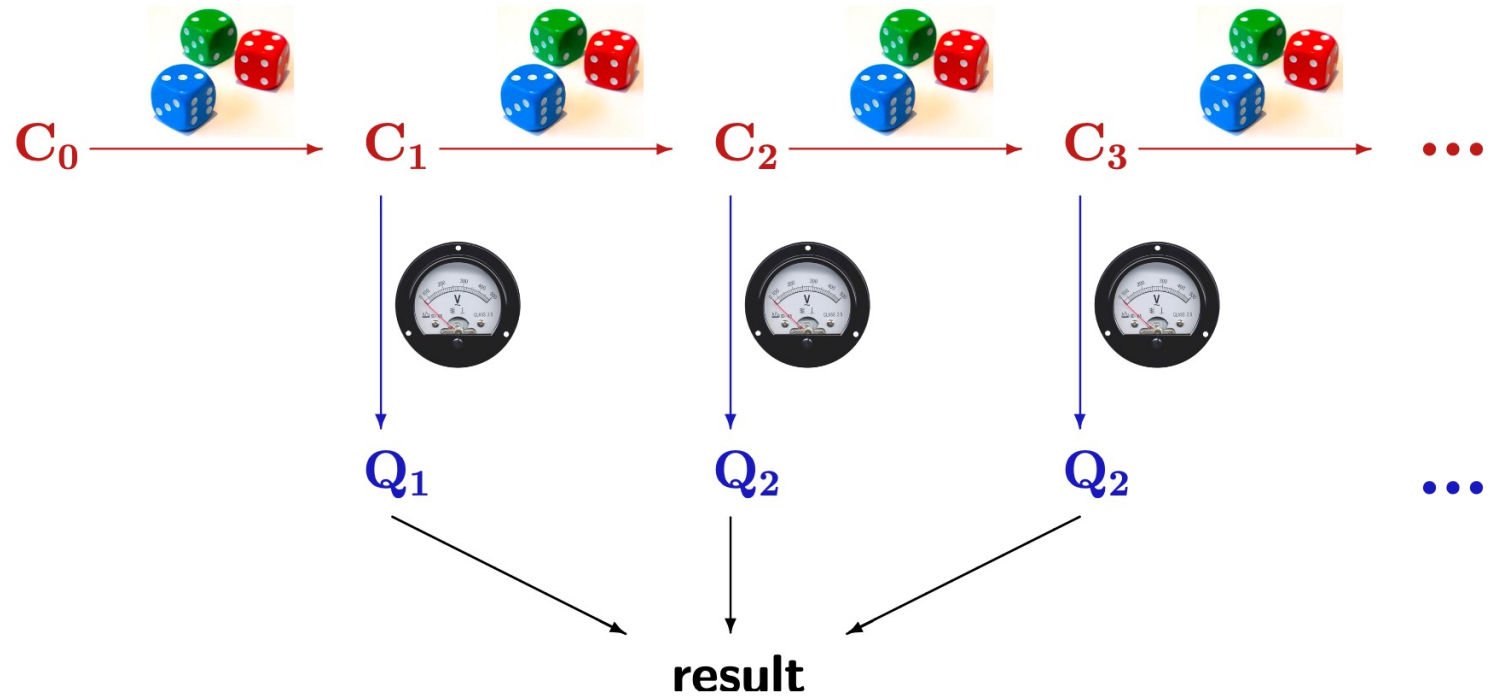
Simulation

HPC / performance

“Measurement”

HPC / throughput

Analysis



Raw data: samples (“ensembles”) of “configurations” $\{ C_i \}$

(An ‘ensemble’ is a SET of ‘configurations’ produced in a single Markov Chain)

- **large** volume (1 ...100 GB \times 1000 ...10000 configs)
- **expensive** to generate (1 . . . 100 million core hours / ensemble)
- **re-usable** in multiple projects / collaborations for different “measurements”

Simulation and ‘Measurement’ is expensive

CPU Obtained in competitive calls (last 3 years) with indication of the approximate operational cost in € assuming 0,01€ per hour standard cost		
EuroHPC (in LUMI) Benchmark grant EHPC-BEN-2022B07-142 (Oct-Dec 2023)	10 million CPU hours	~100K€
EuroHPC (in LUMI) EHPC-REG-2022R03-166 (March 2023 – March 2024)	58 million CPU hours	~580K€
PRACE at PSNC (2 allocations in Eagle) GIDs: 465 and 466	20 million CPU hours	~200K€
PRACE at HLRN (2 allocations in LISE and EMMY)	35 + 20 million CPU hours	~400K€
Joint PASC project at CSCS (Lugano, Switzerland)	20 million CPU hours	~200K€

Kindly provided by our friend Isabel C.

- Is essential to **reuse** already produced configurations.
- In order to be able to do that you need to **find** those configurations based on a known set of meta-data (keys)

Does this remind you of something ?

The International Lattice Data Grid

Objectives

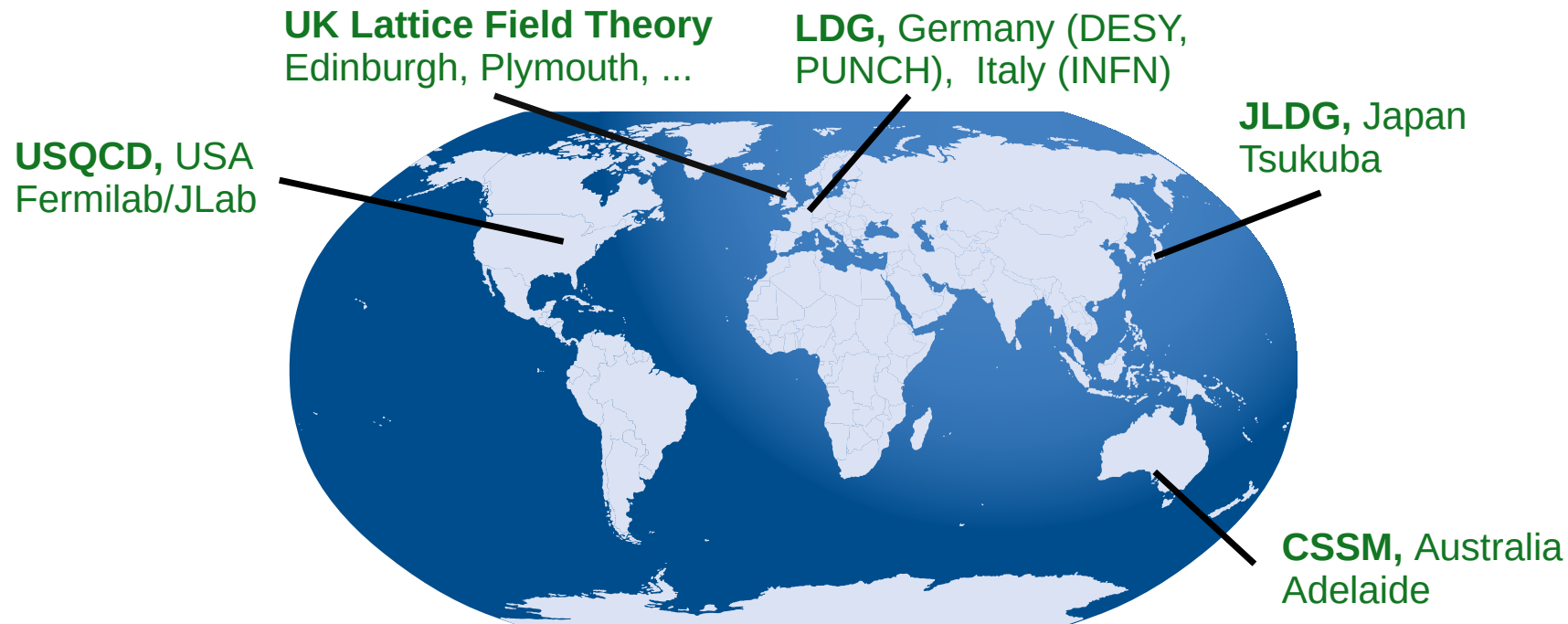
- make raw data sharable and usable for world-wide community
 - ensure basic quality standards for Lattice data management
 - must be convenient for data providers and consumers
 - must support also collaboration-internal sharing
 - follow FAIR-principles
-
- Concepts presented at Lattice conference **2002** Working Groups for Metadata and Middleware
 - Concise and community-wide agreed **metadata schema 2004**
 - 1st generation of **federated services and infrastructure**
 - ... operational since 2007
 - ... but usability and availability **had severely degraded by 2020**
 - **Reactivation and modernization** since 2022 (funding by PUNCH4NFDI)



Basic Concepts of ILDG

ILDG

- Federation of **autonomous** “Regional Grids” (RG)
- **One** Virtual Organisation (VO)
- **Community-wide agreed standards** (QCDml metadata schema, data format, APIs)



Nationale Forschungsdaten Infrastruktur and the EOSC



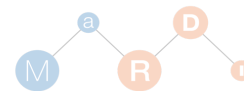
Mandated
Organisation for
Germany



Besides 21 other
German organisations
and 250 Europewide

In the German National Research Data Infrastructure (NFDI), valuable data from science and research are systematically accessed, networked and made usable in a sustainable and qualitative manner for the entire German science system. Up to now, they have mostly been available on a decentralised, project-related or temporary basis. **The NFDI aims to create a permanent digital repository of knowledge as an indispensable prerequisite for new research questions, findings and innovations.**

Natural Science



Engineering Science



Humanities and Social



BERD
@NFDI



Life Sciences

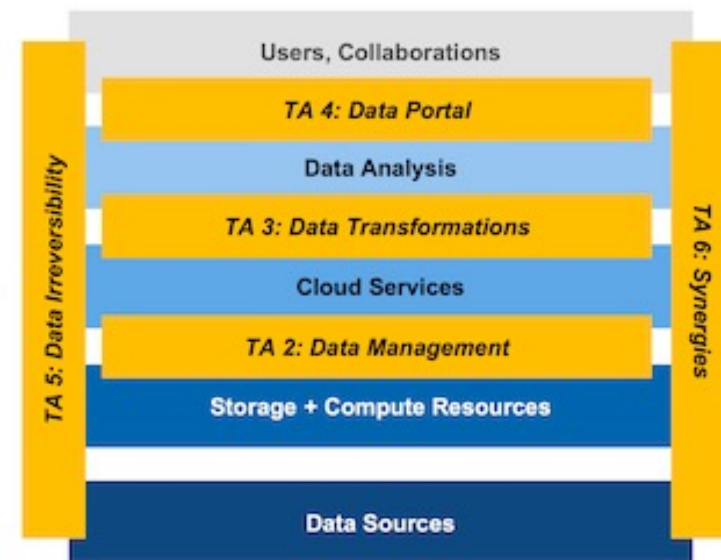
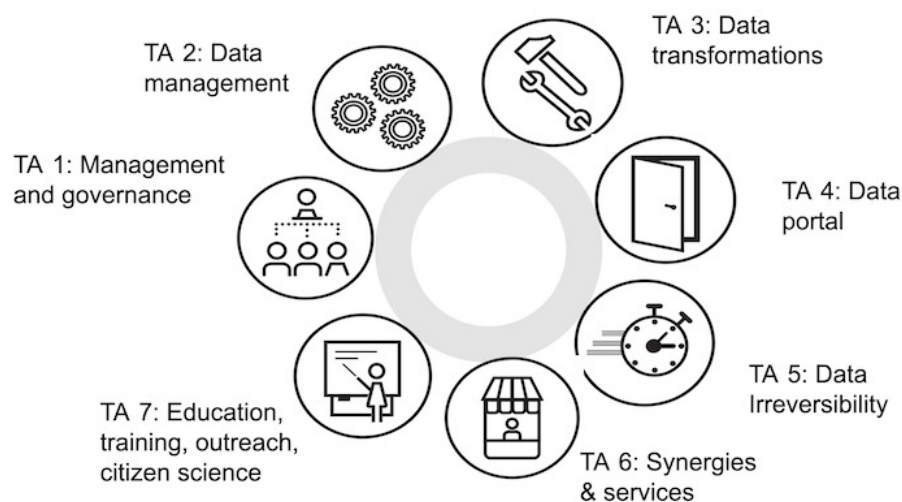


Particles, Universe, Nuclei and Hadrons for the NFDI

Particles, Universe, NuClei and Hadrons for the NFDI

A consortium in the NFDI.

PUNCH science data platform – **the biotope for FAIR and open data** / DRP lifecycles, providing access via portal and AAI.



Basic Concepts of ILDG

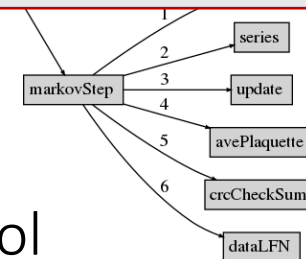
FAIR Principles [F1, A1 F2, R1]

- Globally unique identifier (for configurations and ensembles)
- Rich metadata
 - content/physics – provenance
 - format
 - access policies
 - ...
- standardized formats and APIs

Modular implementation

- leveraging existing infrastructure and middleware (e.g. WLCG)
- plus dedicated Metadata Catalogue and fine-grained access control

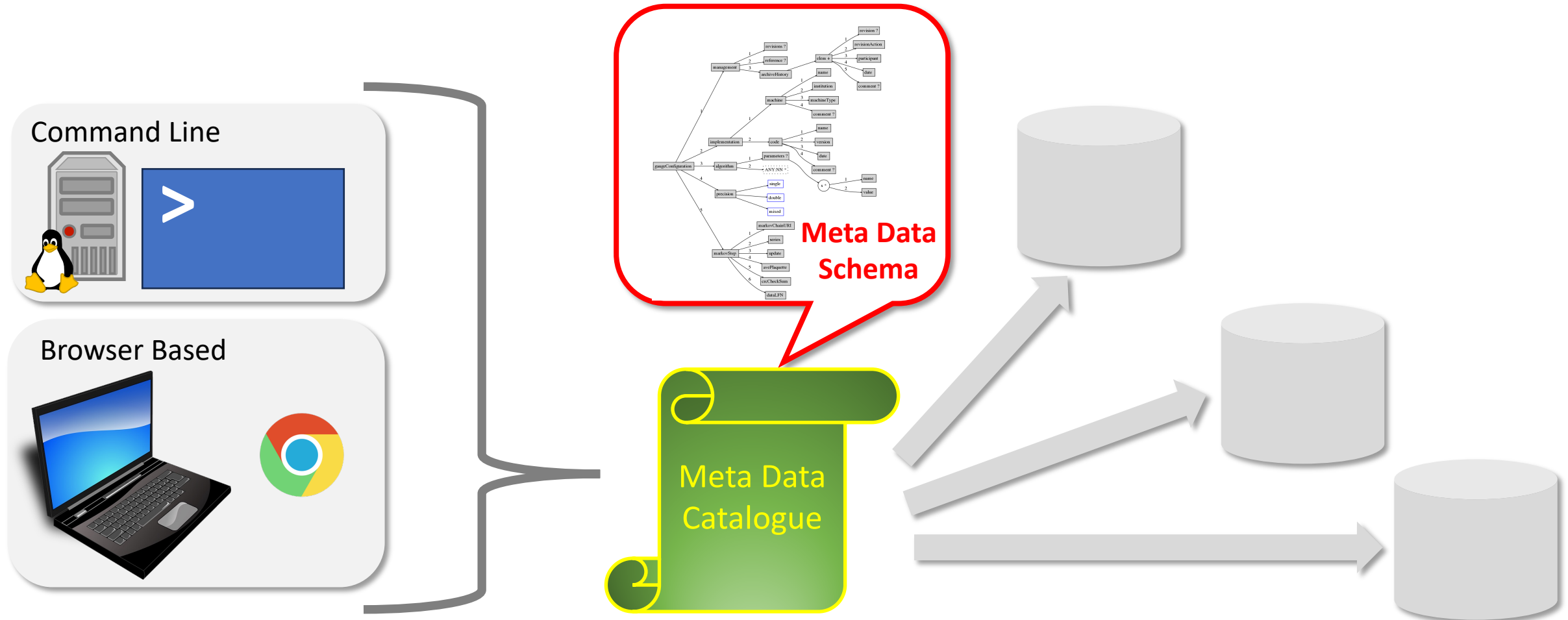
- **F1** (Meta)data are assigned a globally unique and persistent identifier
- **A1** (Meta)data are retrievable by their identifier using a standardised communications protocol
- **F2** Data are described with rich metadata (defined by R1 below)
- **R1** (Meta)data are richly described with a plurality of accurate and relevant attributes



ILDG Metadata

Metadata is stored separately from large data and searchable in catalogue(s) with

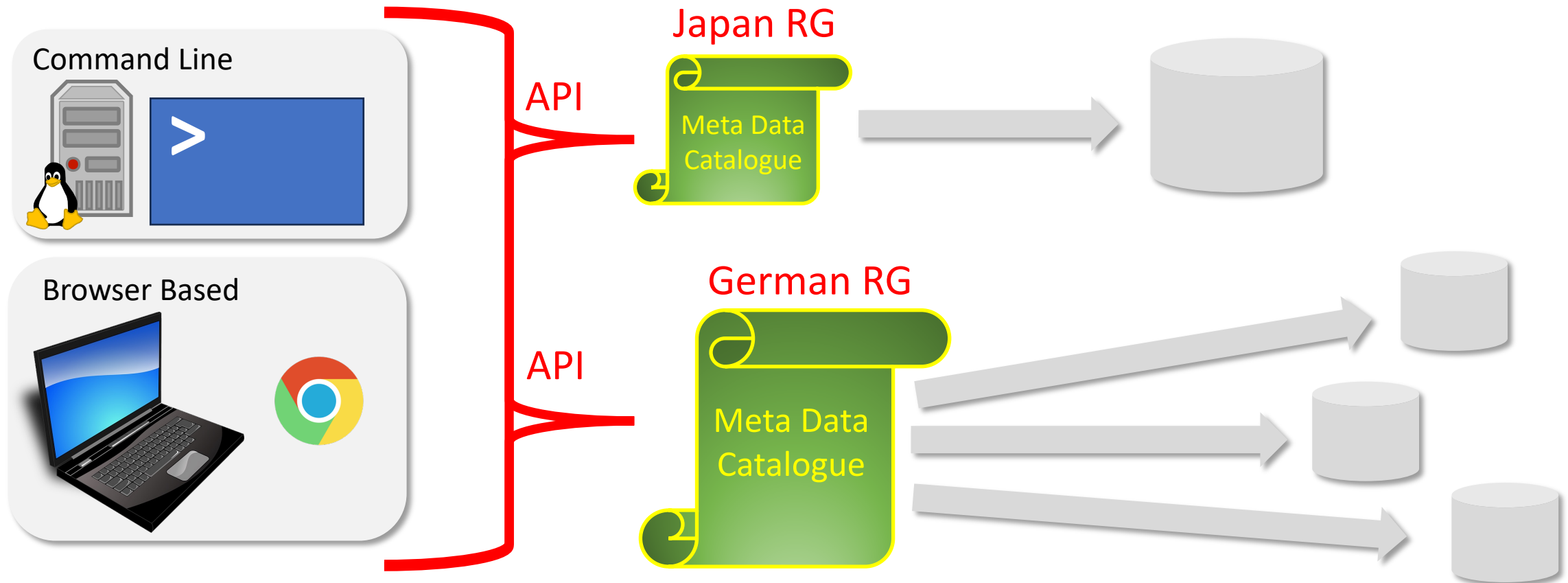
- Concise and extensible XML schema



ILDG Metadata

Metadata is stored separately from large data and searchable in catalogue(s) with

- Concise and extensible XML schema
- **Standardized API**



Interplay between ILDG Services

Services
of ILDG

Website
URL(s) to the MDC Services

VOMS
URL(s) to the FC Services

Meta Data Catalogue

File Catalogue

Storage
Element

Storage
Element

• **MCU**
mgmt
physics
algorithm

• **LFN**
MCU
mgmt
crc
prov
sim

LFN

SURL 1
SURL 2

SURL 'n'

Format
LFN

Format
LFN

Configuration

Configuration

Raw Data

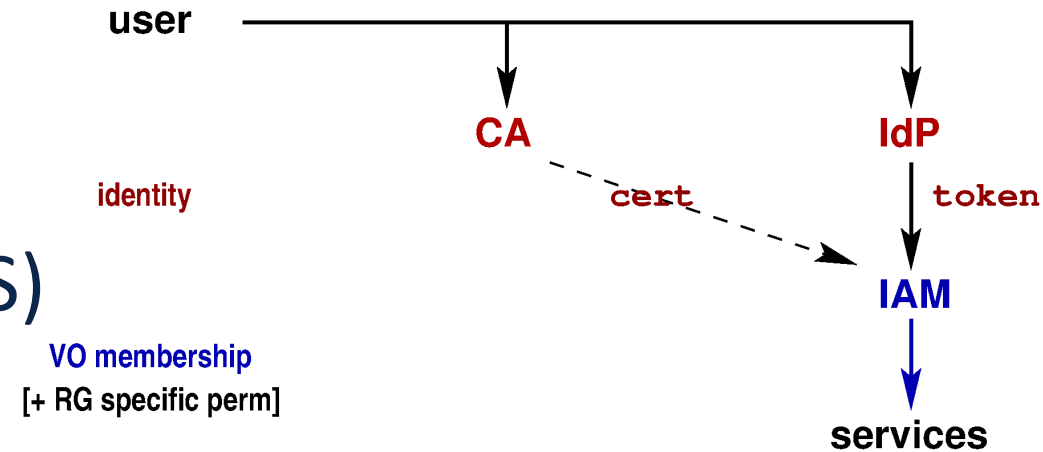
Read Access

Fully Public

Possibly Restricted

Towards ILDG 2.0

- VO user registration: VOMS → IAM
 - new VO policy, GDPR, . . .
- New Metadata Catalogue (MDC+FC+ACS)
- Token-based authentication
 - token exchange flow between MDC and IAM
- Adjustment and extension of metadata schema
- Extension of data format (HDF5)
- Update and improvement of clients
 - for searching, markup, and upload
- Support for data publishing
 - DOI registration, generation of landing pages, harvesting

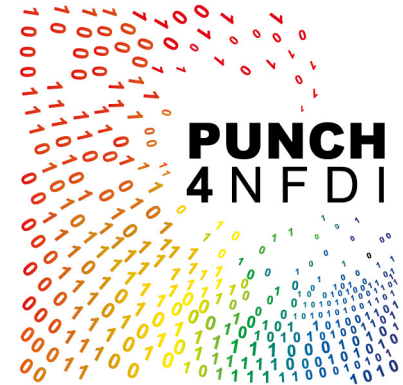


New Implementation of MDC and FC

Features

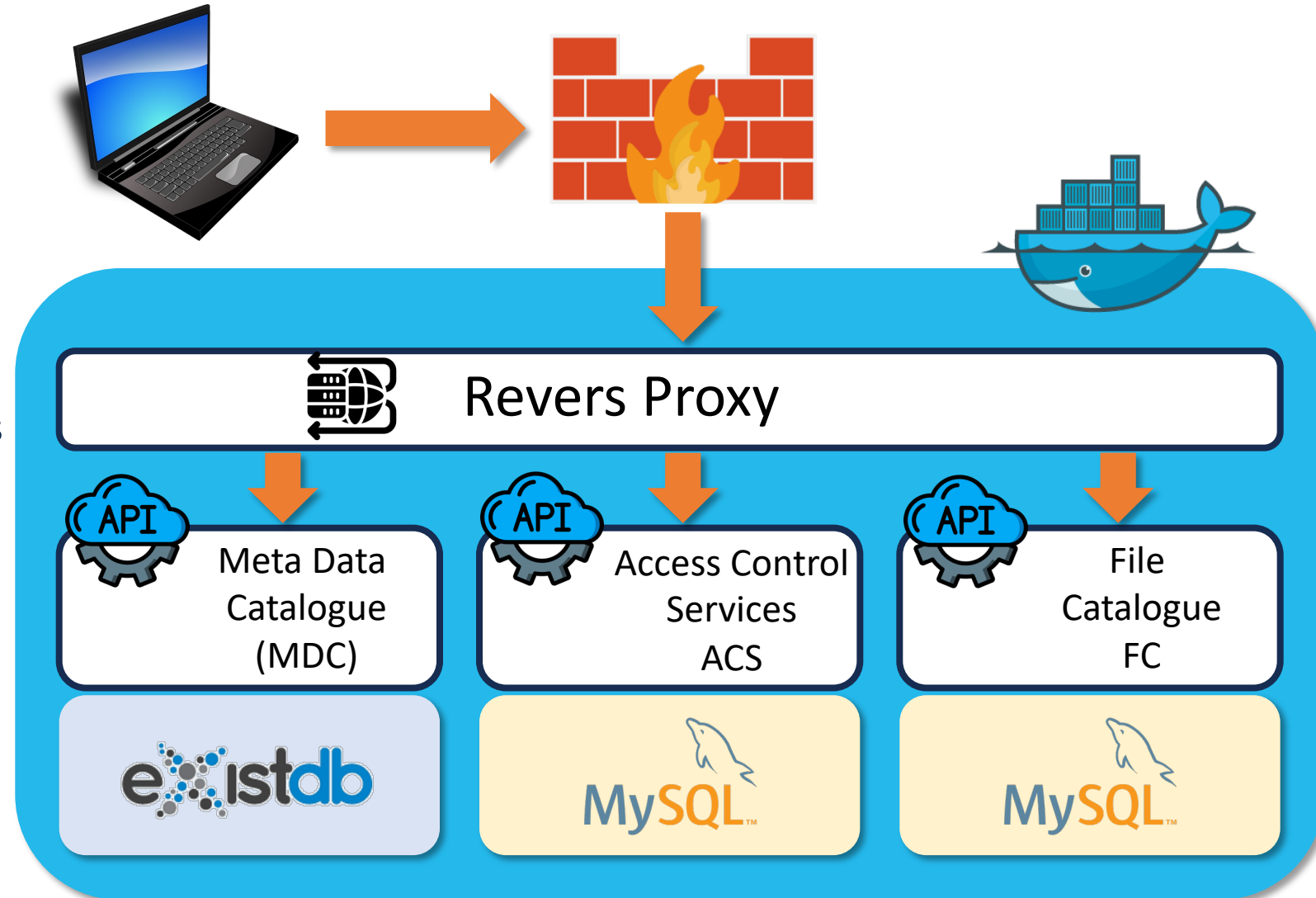
- **Configurable** with support for multiple metadata collections / schemas
- **Separated File Catalogue** included
 - Useful if **external File Catalogue** exists (e.g. RUCIO)
- Includes Attribute Service for **fine-grained access control**
 - for individual resources/identifiers, associated with independent projects
- new **REST API** (see online documentation [MDC](#), [FC](#), and [ACS](#))
- simple **deployment** (Docker swarm, Kubernetes in preparation)

➤ re-usable for other regional grids or for non-lattice data



Architecture of MDC/FC/ACS

- Configurable access policies
- Independent (and optional) use of MDC/FC/ACS functionalities, e.g.
 - only MDC or
 - only FC
 - also without ACS if write access is only done on server-side



Fine grained Access Control: Access to MDC or FC



or CLI

Indigo Identity and
Access Manager

Meta Data and
File Catalogue

Access Control
System

User

IAM

MDC / FC

ACS

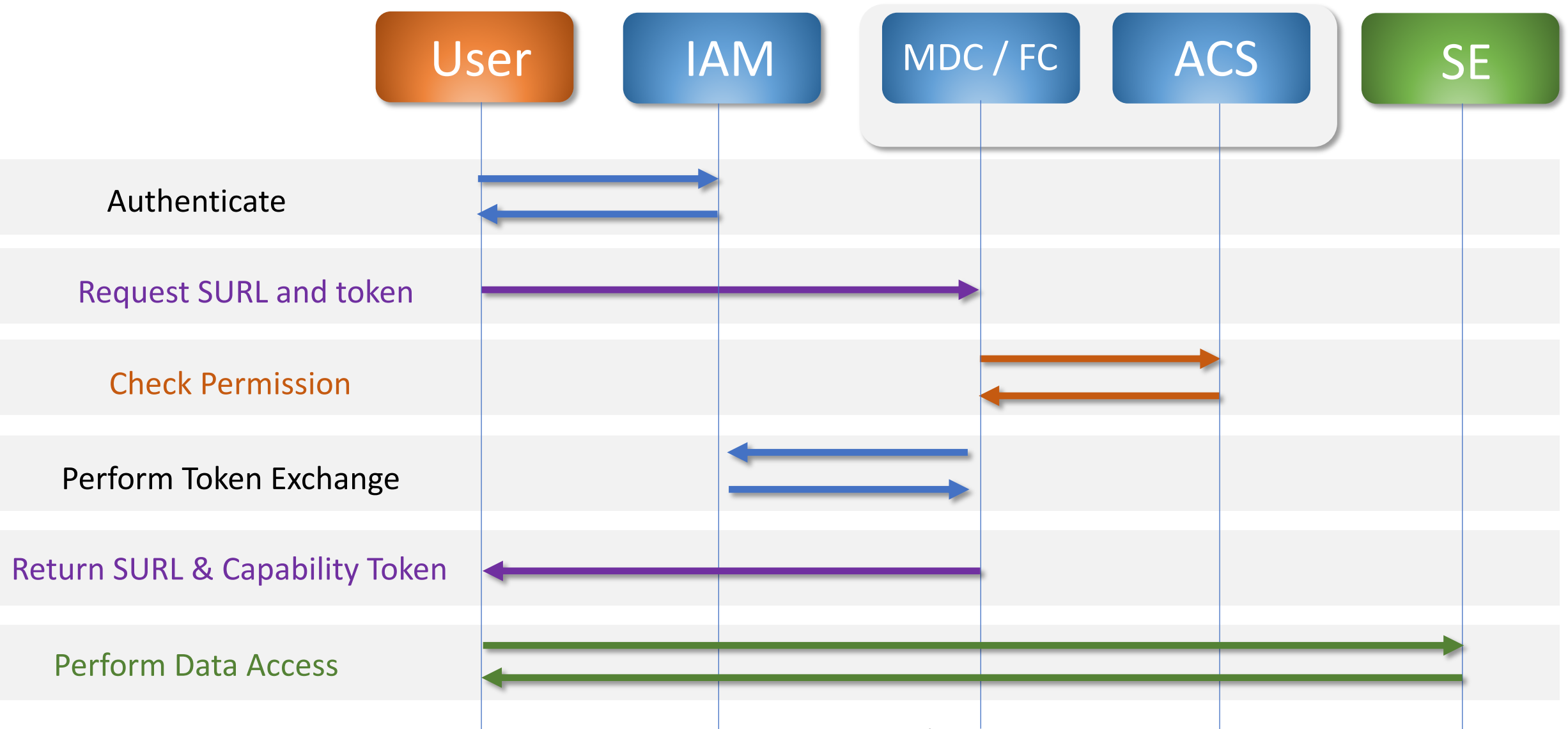
Authenticate

Access Request

Check Permission

Access Response

Fine grained Access Control: Access to Storage Element (Data)



Use Cases

Consumer

Provider

Collaboration Internal

lfind: search in metadata catalogue
lget: download data and metadata

lpack: generate markup (*) and pack data
linit: register ensemble metadata
lput: upload config data and metadata

Community wide

- Optionally also use common search engines
- Cite DOIs when using published data

- Optionally register DOI and generate landing page
- Drop access restriction flag
- Receive data citation record

(*) Trivial if information is already collected during production!

Summary and outlook

- Two Regional Grids operational (Europe, Japan)
- In progress: transition to tokens and user-friendly clients
- Applications beyond Lattice QCD?

Finish

