International Lattice Data Grid

DMA ST1 Meeting

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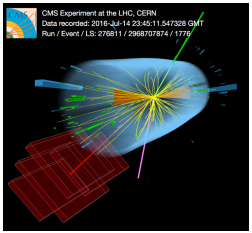
QCD on the Lattice

Quantum Chromodynamics (QCD)

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

where
$$\langle Q \rangle = \int_C e^{-S(C)} \cdot Q(C)$$

- **C** = gluon (quark) field configuration at each point in 4d space-time
- **S** = classical action ($\leftrightarrow$ field equations)



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

$$\langle Q \rangle \sim \sum_{i=1}^{N} e^{-S(C_i)} \cdot Q(C_i)$$

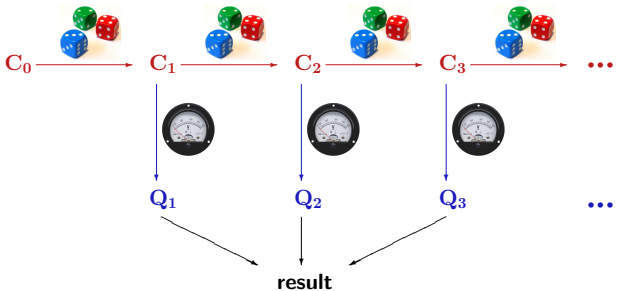
$$\begin{pmatrix} \text{sample size } N & \to & \infty, \\ \text{lattice spacing} & \to & 0, \\ \text{phys volume} & \to & \infty, \\ \text{masses } m & \to & m_{phys} \end{pmatrix}$$

Lattice QCD: Simulation Workflow and Data

Simulation
HPC / performance

"Measurement"
HPC / throughput

Analysis



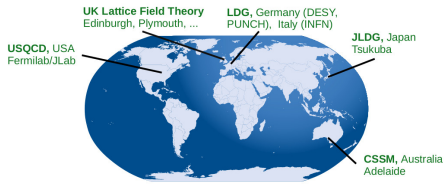
"Raw" data = samples ("ensembles") of gluon (gauge field) "configurations" $\{C_i\}$

- low "event rate": 1 config / 30'000 core hours → massive parallelization
- large volume: 1 ... 100 GB × 1000 ... 10000 configs → O(PB)
- expensive to generate: 1 ... 100 million core hours / ensemble
- re-usable in multiple projects / collaborations for different "measurements"

International Lattice Data Grid (ILDG)

Community effort to share expensive primary data:

- proposed at Lattice conference 2002
- community-wide agreed **metadata schema** 2004
- first services operational $\approx$ 2007



Organization:

- federation of autonomous "Regional Grids"
- forming a single Virtual Organization (VO)
- 2 Working Groups (metadata and middleware) + Board

Basic Concepts:

- ILDG defines standardized metadata schema, file-format, API [hpc.desy.de/ildg]
- Regional grids (with specific policies, technologies, resources, ...) provide catalogue services + storage

  E.g. LDG in Europe makes to a large extent also use of WLCG technology and services

Towards ILDG 2.0

Situation around 2020

- ✘ Usability of ILDG services had severely degraded
- ✘ ILDG had started 10 years before formulation of FAIR principles

Aims for ILDG 2.0

- ➜ Become fully FAIR-compliant
- ➜ Re-activate and organize regional grids
- ➜ Modernize concepts and basic gearbox
- ➜ Explore support for non-lattice use-cases

Critically relied on PUNCH4NFDI funding for 2y of a professional SW developer

FAIR principles for scientific data management and stewardship

Findable
Accessible
Interoperable
Reusable

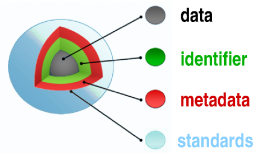
force11.org
⋮
Wilkinson 2016
⋮
go-fair.org

- required by funding agencies

EU Commission 2016

- 15 concise principles formulated in Wilkinson 2016
  - globally and unique persistent identifiers (F1)
  - rich metadata (F2)
  - metadata is registered and can be searched and harvested (F4)
  - authentication/authorization procedure where necessary (A1.2)
  - metadata accessible even when data is no longer available (A2)
  - ...

  41 detailed indicators in FAIR Data Maturity Model



- guiding principles (not implementation)

FAIR data: a local implementation

Logical organization as a **database:**

- ❒ each FAIR data object becomes entry (row) in a database (table) with 3 fields (columns)

  ➜ retrievable by ID (A1) and searchable by metadata (F4)

- ❒ mint **persistent identifiers** (ID)
- ❒ define appropriate **metadata schema** and storage format
- ❒ possibly implemented just through a local POSIX file system

  i.e. buy a big disk and use standard tools: `ls`, `grep`, `find`,  , ...

- ❒ additional **access control** mechanisms are required for "sharing" of data

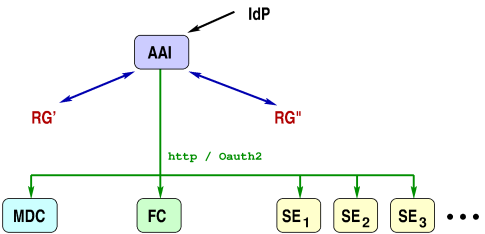
N.B.: Technically, ILDG could be implemented by a **single central** infrastructure

FAIR data: a distributed implementation

For **large** data objects or volumes: need to split (physical) storage of metadata and data

➜ **distributed** implementation: typically by distinct **web services** (not pages):

- Authentication and Authorization (AAI)
- Metadata Catalogue (MDC)
- File Catalogue (FC)
- Storage Elements (SE)



where

- separate MDC and SE becomes mandatory for large data objects (cost of search)
- multiple SE may become mandatory in practice (replication, funding, ownership)
- FC becomes mandatory if there are multiple SE or varying storage locations (SURL)

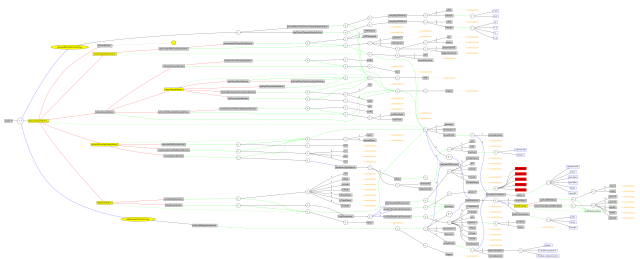
Status of ILDG 2.0

- ✔ Revision of ILDG specifications for metadata schema, file format, and API of catalogue services [arXiv:2502.09253]
- ✔ Re-factored catalogue services
  - Metadata Catalogue: ID $\longleftrightarrow$ metadata
  - File Catalogue: SURL $\longrightarrow$ ID (LFN)
  - Access Control Service: user $\longleftrightarrow$ (meta-)data
- ✔ New user registration and VO management by Indigo IAM
- ✔ Complete transition to tokens (replacing X.509 grid certificates)
  ➜ enable fine-grained access control to metadata and data
- ✔ Prototypes for optional add-on services/interfaces
  ➜ assemble flexible and modular distributed RDM systems

ILDG Metadata Schema

- Rich and community-agreed schemata for descriptive (scientific) metadata
  - physics
  - algorithm
  - provenance
  - data management

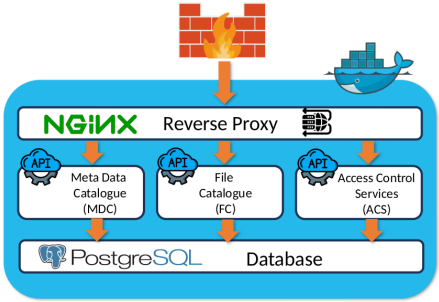
  ($\approx$ 350 elements, vs. $<$ 100 of DataCite)

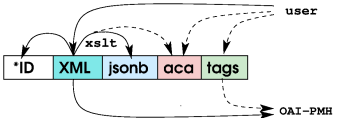


- XML remains preferred format
  - W3 standard
  - rigorous grammar (XSD) for creation and validation of metadata
  - powerful and complex query technologies (Xpath, Xquery)
  - many tools and libraries for processing XML documents

Re-factored Metadata Services

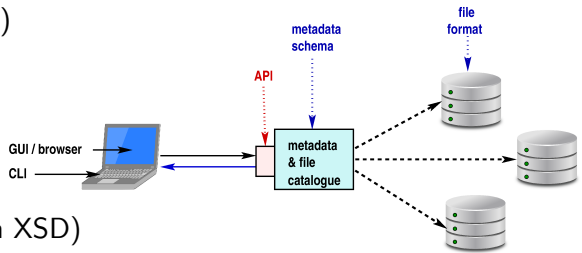
- Simple containerized deployment
  (currently at Bielefeld, DESY, Jülich, Plymouth, Tsukuba)
- Metadata Catalogue:
  - multiple metadata collections, each with freely configurable schema (XSD)
  - Xpath and "quick-search" queries
    ↓ XML ↓ jsonb
- File Catalogue:
  - efficient reverse look-up of Storage URL → ID
    (data may be moved or replicated)
- Access Control Service





Interoperable ILDG Services and add-on Interfaces

- Each regional grid autonomously implements and operates basic ILDG services
- Interoperable by ILDG-wide standards
  (metadata schema, file format, REST API)
- Optional add-on services and interfaces
  - file transfer service (FTS)
  - metadata harvesting (OAI-PMH)
  - fine-grained access control
  - markup and query GUI (parametric in XSD)
  - ...



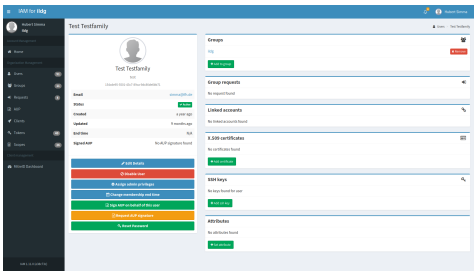
(see e.g. MDC index)

Identity and Access Management (IAM)

ILDG Middleware Working Group tested and evaluated different solutions (incl. Unity AAI)

➜ Dedicated Indigo IAM instance at INFN-CNAF

- user and group management
- enforce VO-specific policies and LoA
- registered as eduGAIN Service Provider
- OIDC provider and OAuth2 token issuer
- flexible OAuth2 client registration
- flexible scope configurations (+ policy engine)



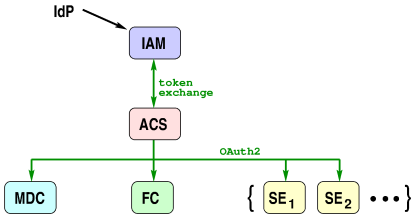
☛ Administrative and technical advantage of a dedicated (community-specific) instance:

IAM as a Service!

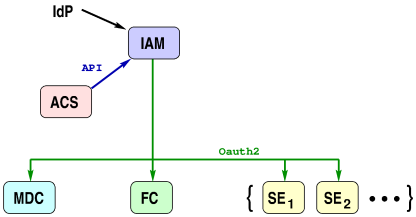
Access Control Service (ACS)

- 3rd "catalogue" for administrative metadata
  - hierarchical delegation (admin → project → groups/users)
  - optional group management (GDPR concerns!)

- ACS in front of IAM



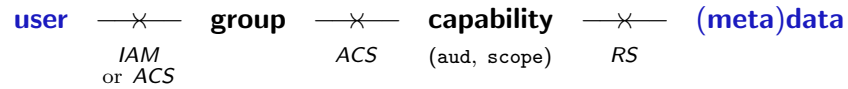
or beside/behind of IAM



☛ Setup of ILDG seems in certain aspects ahead of (or interesting for) other experiments

Attribute-Based Access Control (ABAC Model)

- Policy **enforcement** points → **distributed** Resource Servers (RS = MDC, FC, SE)
- Policy **decision** point → **central** Access Control Service (ACS)
- Break-up the huge user-data relation into smaller many-to-many relations



- Path matching [WLCG Common JWT Profiles 1.0]

SURL = `https://dcache.somewhere.net:2880/a/b` **/c/d**

OAuth2 token:

scope (capability)	access
`storage.read:/`	permit
`storage.read:/c`	permit
`storage.read:/c/d`	permit
`storage.read:/x`	deny
`storage.read:/c/y`	deny

Outlook

- ❒ Fix loose ends and minor issues
  (slowed down without SW developer, now working at CTAO)
- ❒ Start of massive uploads
  ($\approx$ 8 PB by 14 collaborations, see Lattice2024)
- ❒ User tools and training
  (clients, documentation, GUI, hands-on workshop)
- ❒ Setup of data publishing process
  (e.g. with DOI minting via Zenodo or PUBDB)
- ❒ Synergies within and beyond PUNCH4NDFI to exploit and maintain ILDG-like setup
  - Storage4PUNCH, Compute4PUNCH, InterTwin
  - Radio astronomy (GLOW)
  - CTA
  - ...