

Database Solutions for Research Data Management



RDM Summer School Gajendra Doniparthi 19 July 2023



Research Data Management

Data Collection

Organization

Storage

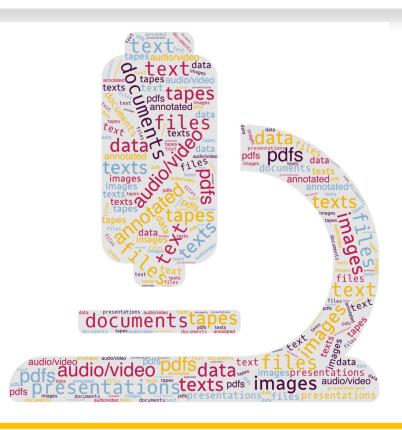
Preservation

Publication



Types of research data

- Images
- Text
- Annotated Texts
- Documents
- Audio/Video tapes
- Presentations
- PDFs
- Data Files ...





Fair Data vs. Open Data

VS.

- Findable
- Accessible
- Interoperable
- Reusable

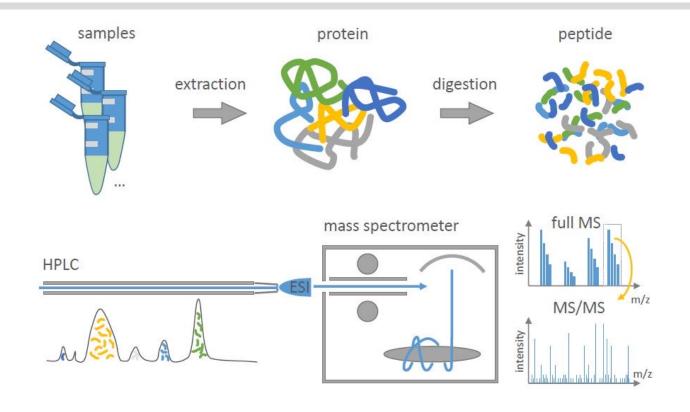
- Openly accessible
- Exploitable
- Editable
- Sharable



Research workflows are often complex!

Proteomics workflow

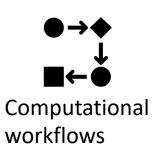






Complex workflows mean complex sets of data to manage.















DataPLANT project solve the complexity through ARCs.







Annotated Research Context (ARC)

Reproducibility

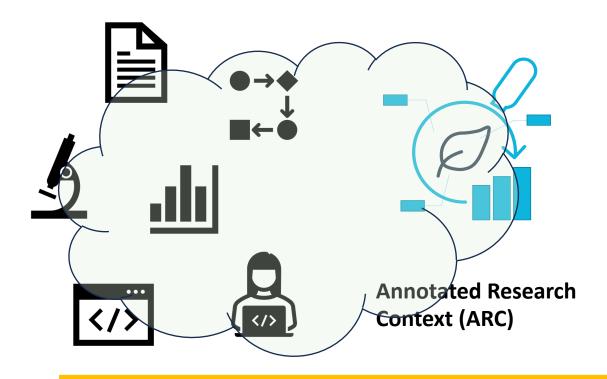
Interoperability

Forward data to **Public Repositories**

FAIR Principles



From the outside, everything is nothing but data!







How to search and explore the Research Data?

Identification

- File types.
- Metadata and raw data files (runs, workflows)
- X-references.

Data Standardization

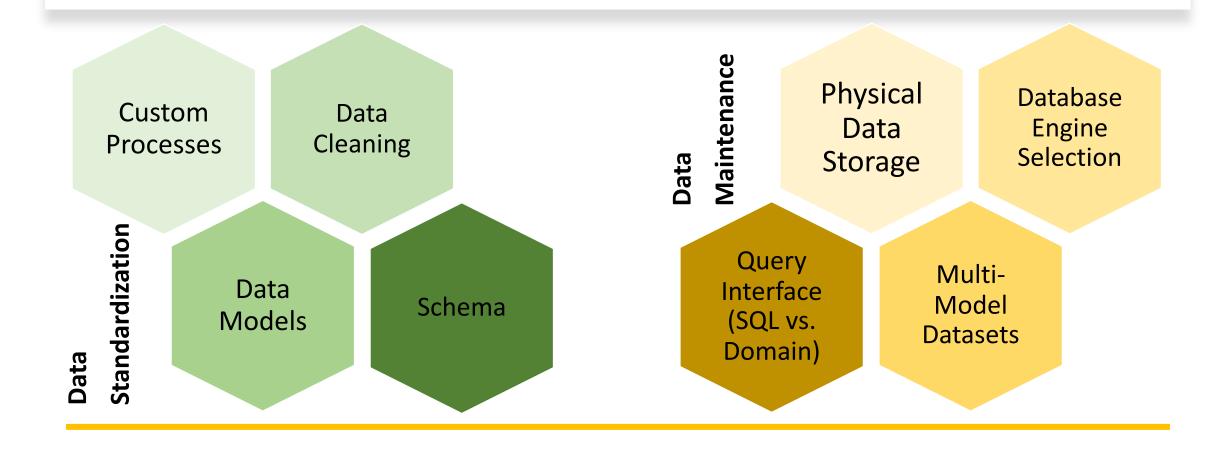
- Standard formats and data model selection.
- Data cleaning & Transformation.

Maintenance

- Physical vs. Virtual
- Databases -> Data Lakes.
- Data Indexing.
- Query processing.



What are the challenges?





There are quite a few data models in practice.









Document







Query Interface plays an important role.

- Useful to hide the heterogeneity of the data sources.
- Domain query model vs. standard query model.
- SQL vs. No-SQL
- Client-interfacing for query execution.



Polystore Systems can be one of the database solutions.

- Provides an integrated view on multiple data sources.
- Each storage engine may have different data model.
- Query interface to access multiple sources.
- Splits input query into multiple sub-queries.



Distributed Query Processing Frameworks are different.

- Open-source SQL query engine for Big Data Exploration
- Can access multiple data sources at once
- SQL query interface
- Schema-free JSON model



Can Data Lakes be also one of the solutions?

- Ability to ingest and store data in the form of structured, semi-structured or unstructured.
- Three logical phases -> Ingestion, Maintenance and Exploration
- Data standardization and modeling techniques.
- Advanced query languages and Indexing capabilities.



Moving physical data from ARCs to a Database solution

Identification

- Identify the files to be processed.
- Capturing metadata.
- Automatic schema generation.

Data Transformation

- Standard data model / multimodel
- Data cleaning.
- Data update captures.

Ingestion & Exploration

- Bulk loading of single/multi-model data.
- Data Indexing.
- Query processing / exploration.

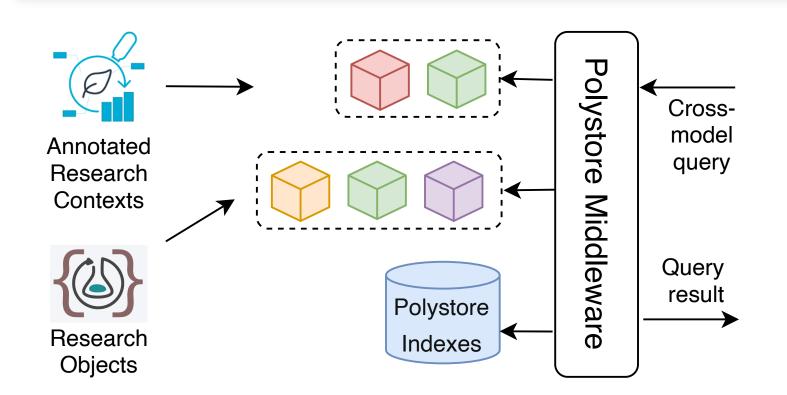


The role of Docker containers in in-situ query processing

- Docker helps query the data directly from individual ARCs.
- Helps develop an on-demand data exploration platform.
- Easy to integrate ARCs with Distributed Query Processing frameworks.
- No need to maintain huge volumes of Research Data in physical database systems.



Should we re-design the wheel?



- 1. SQL Query Interface
- 2. Custom Optimiser
- 3. Custom Adaptive Indexing
- 4. Designed for Cross-omics



Questions





Distributed Query Processing Framework - Hands-on









Cast & Crew



Document









Apache Drill System Docker Setup

- Clone the repo gdoniparthi/summerschool from GitHUB
- Docker pre-requisites (Docker desktop, Docker compose)
- Bootstrap the docker network (docker compose up d).
- Setup PostgreSQL and MongoDB with Apache Drill.
- Execute test queries.



TMDB Dataset Description

Table "public.mo Column Type budget double precision genres json homepage character varying id integer keywords json original_language character varying original_title character varying overview character varying popularity character varying production_companies json production_companies json release_date character varying revenue double precision runtime double precision spoken_languages json status character varying tagline character varying title character varying vote_average double precision vote_average double precision vote_ount integer		
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vote_average double precision	tagline	character varying
	title	character varying
vote count integer	vote_average	double precision
	vote_count	integer

Column	Table "publ Type
genre genre_id movie_id	character varying integer

Column	Table "publ Type +
keyword	character varying
keyword_id	integer
movie_id	integer

```
[movies> db.casting.findOne()
{
    _id: ObjectId("64b6e584c887f773faf3eddb"),
    cast_id: 4,
    character_name: 'Col. Quaritch',
    gender: 2,
    name: 'Stephen Lang',
    order_id: 3,
    movie_id: 19995
}
```

```
[movies> db.crew.findOne()
{
    _id: ObjectId("64b6e58c22f1b9739fe169aa"),
    department: 'Editing',
    crew_id: 1721,
    name: 'Stephen E. Rivkin',
    job: 'Editor',
    movie_id: 19995
}
```