Updates on iRODS Data Repository Service Adapter

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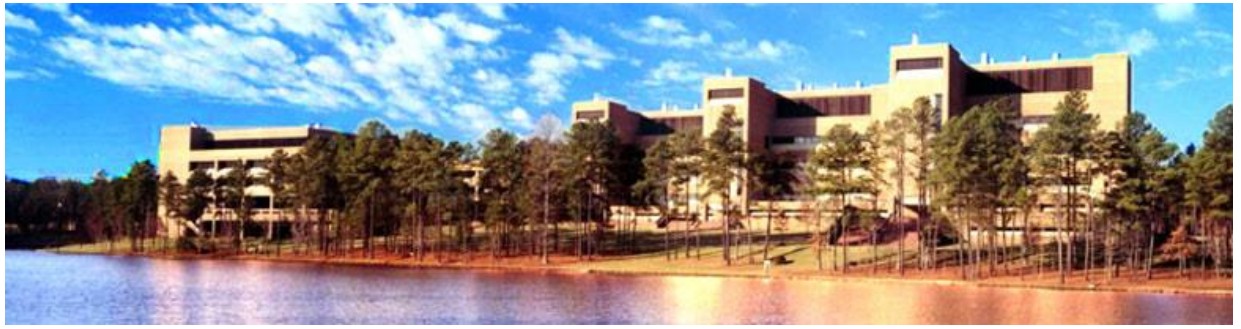
Sofware and AI/ML Tools for Computational Toxicology

"Computational toxicology is a subdiscipline of toxicology that aims to use the mathematical, statistical, modeling, and computer science tools to better understand the mechanisms through which a given chemical induces harm and, ultimately, to be able to predict adverse effects of the toxicants on human health and/or the environment."



Rusyn I, Daston GP. Computational toxicology: realizing the promise of the toxicity testing in the 21st century. Environ Health Perspect. 2010 Aug;118(8):1047-50. doi: 10.1289/ehp.1001925. Epub 2010 May 18. PMID: 20483702; PMCID: PMC2920091.

Current Activities

IRODS at NIEHS

iRODS has been in use for several years to preserve NGS data

- **20,075,498 raw run files**
- **328,426 processed FASTQ files**

All runs have full metadata at the project and sample level

Challenges we Face

Standards, Sustainable Software Practices, Cloud-ready, FAIR Research Software

Data Sharing and Federation

- Increasingly data-driven
- Multi-institutional data collaboration
- Hybrid cloud/on-prem computing
- Heterogeneous data, institutional, specialized and generalist repositories
- Handling PHI/PII, maintaining privacy

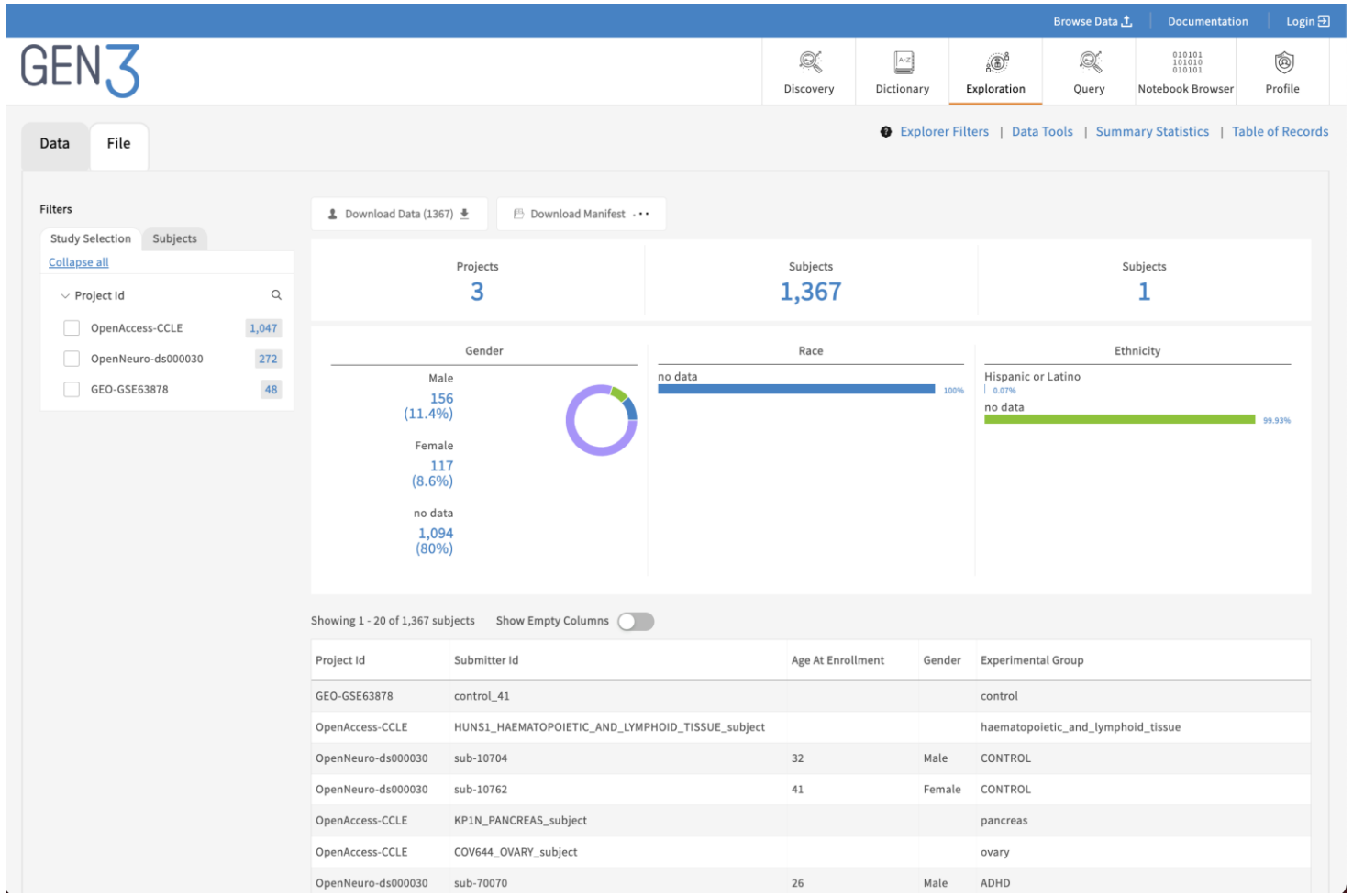
AI and Machine Learning

- Systematic Review, extracting data from reports and publications
- ToxPipe - Interacting with and discovering relationships in diverse data sources

Elevating the role of Research Software Engineers

CHORDS Project

- Intersection of Climate and Health (Wildfires) - A Data Catalog
- Gen3 Platform (Biomedical Research Hub)
- An attempt to better align NIEHS with NIH platforms/standards
- **Data Grid, Data Commons, Data Mesh**



Data Sharing Architectures (As defined by Gen3 developers)

Data Commons

Software platforms that co-locate:

1. curated data
2. cloud-based computing infrastructure, and
3. commonly used software applications, tools and services to create a governed resource for managing, analyzing and sharing data with a research community.

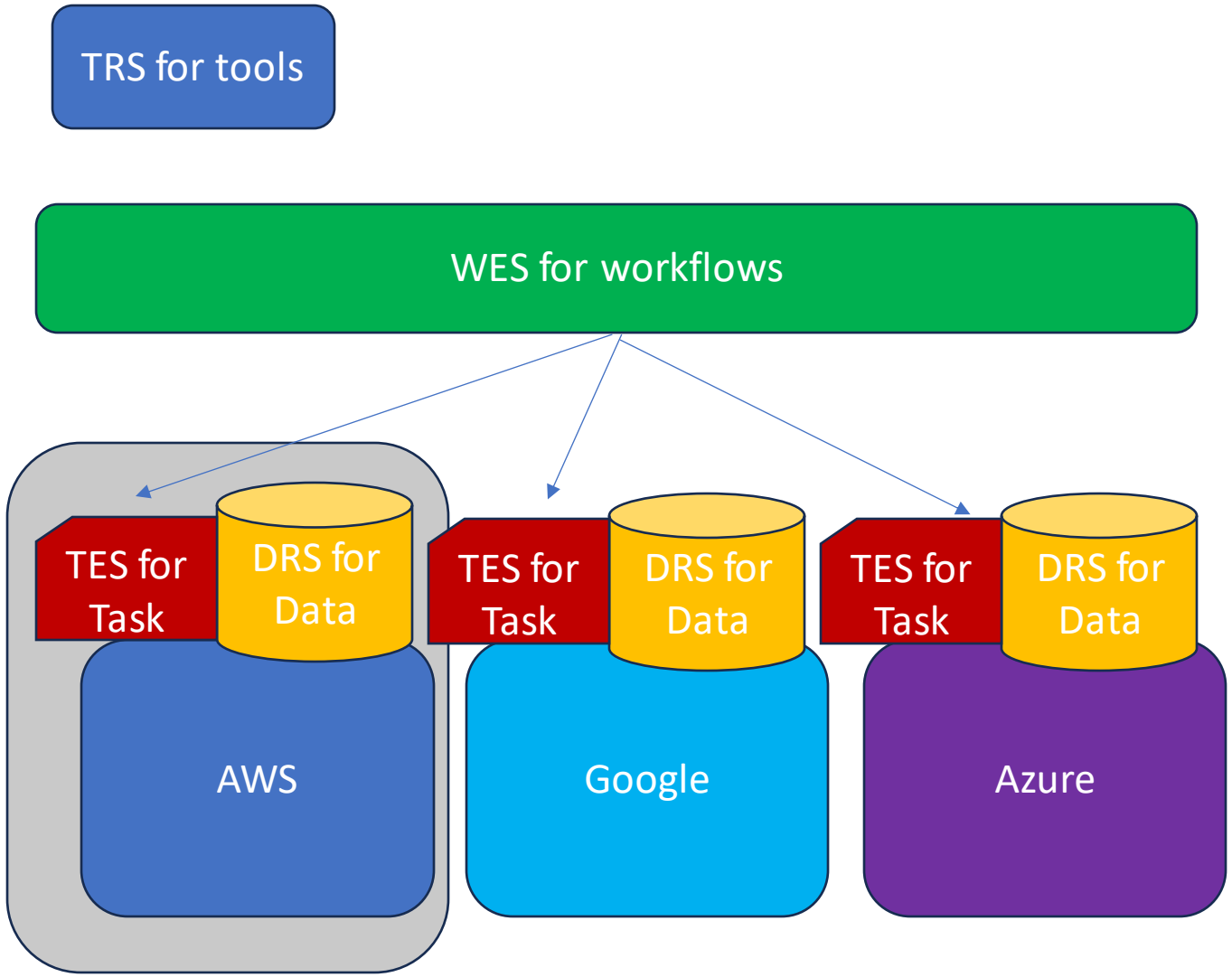
Data Mesh

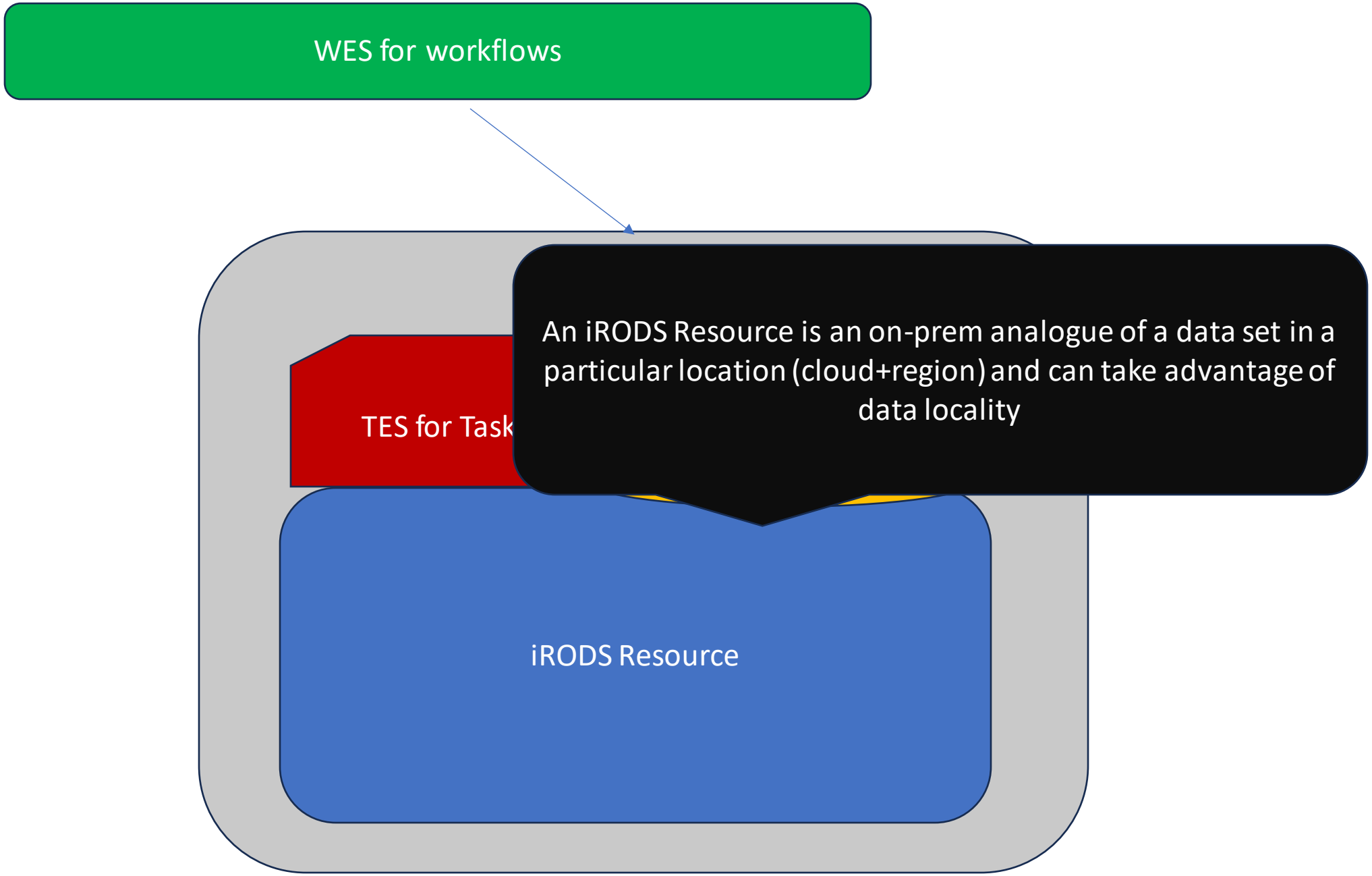
(aka data ecosystems) integrate multiple data commons, computational platforms, and other cloud-based resources operated by different organizations, along with a hybrid governance framework, and enable the management, discovery, analysis and sharing of data.

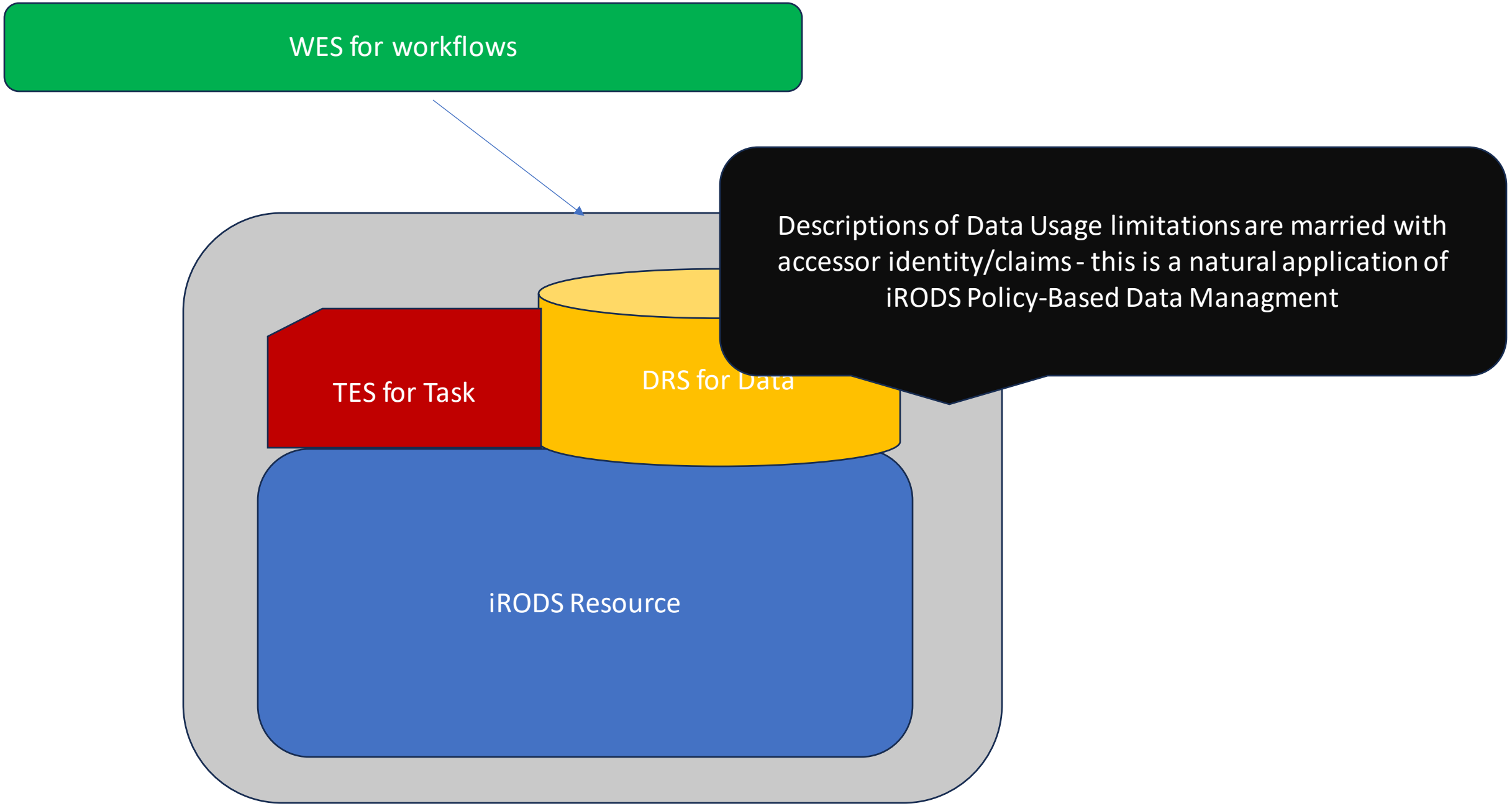
Bob Grossman. "How to Build a Data Mesh Using Gen3," May 1, 2023. https://gen3.org/community/events/Gen3%20Forum%20May%201%202023%20-%20Data%20Meshes.pdf.

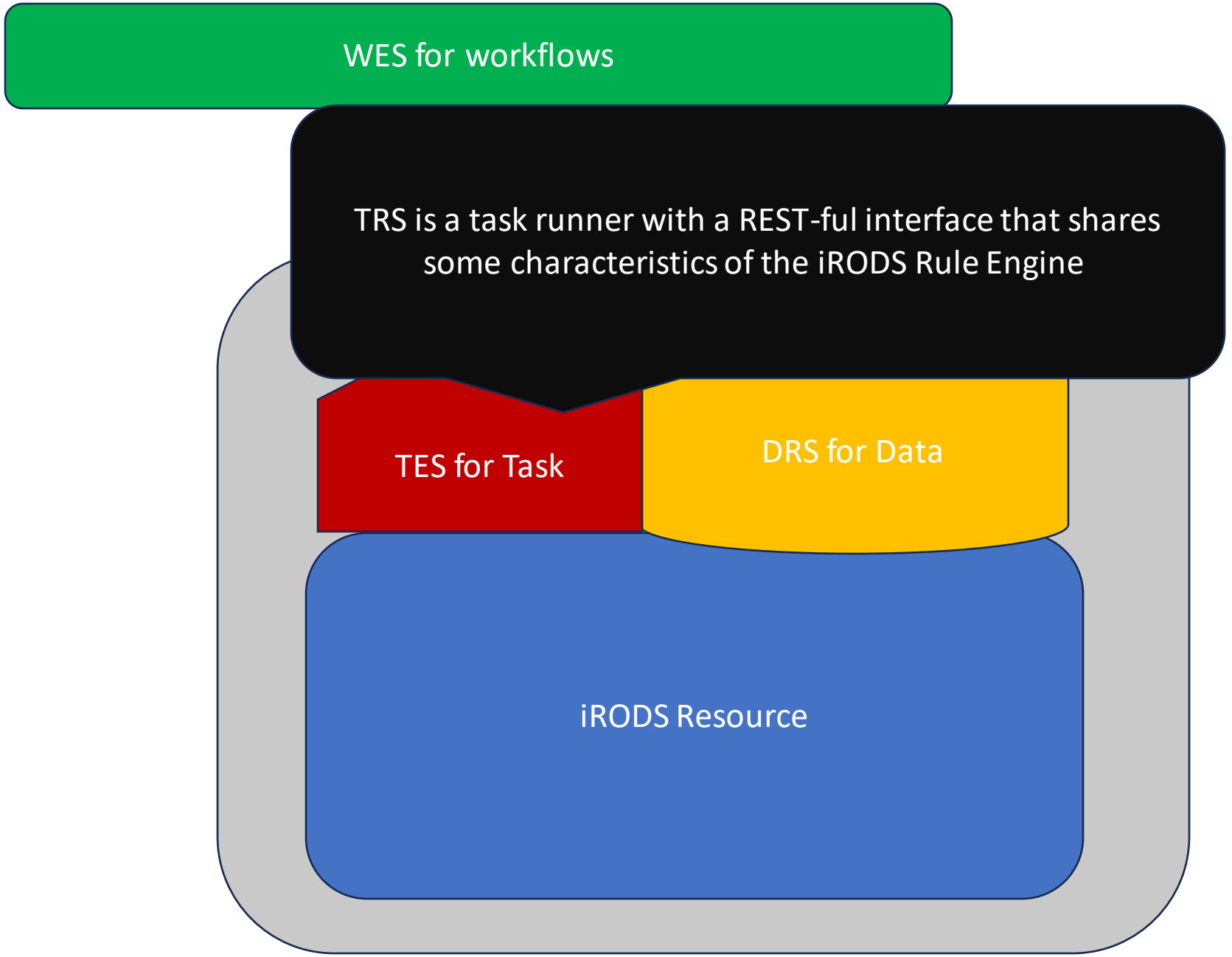
Federated Analysis

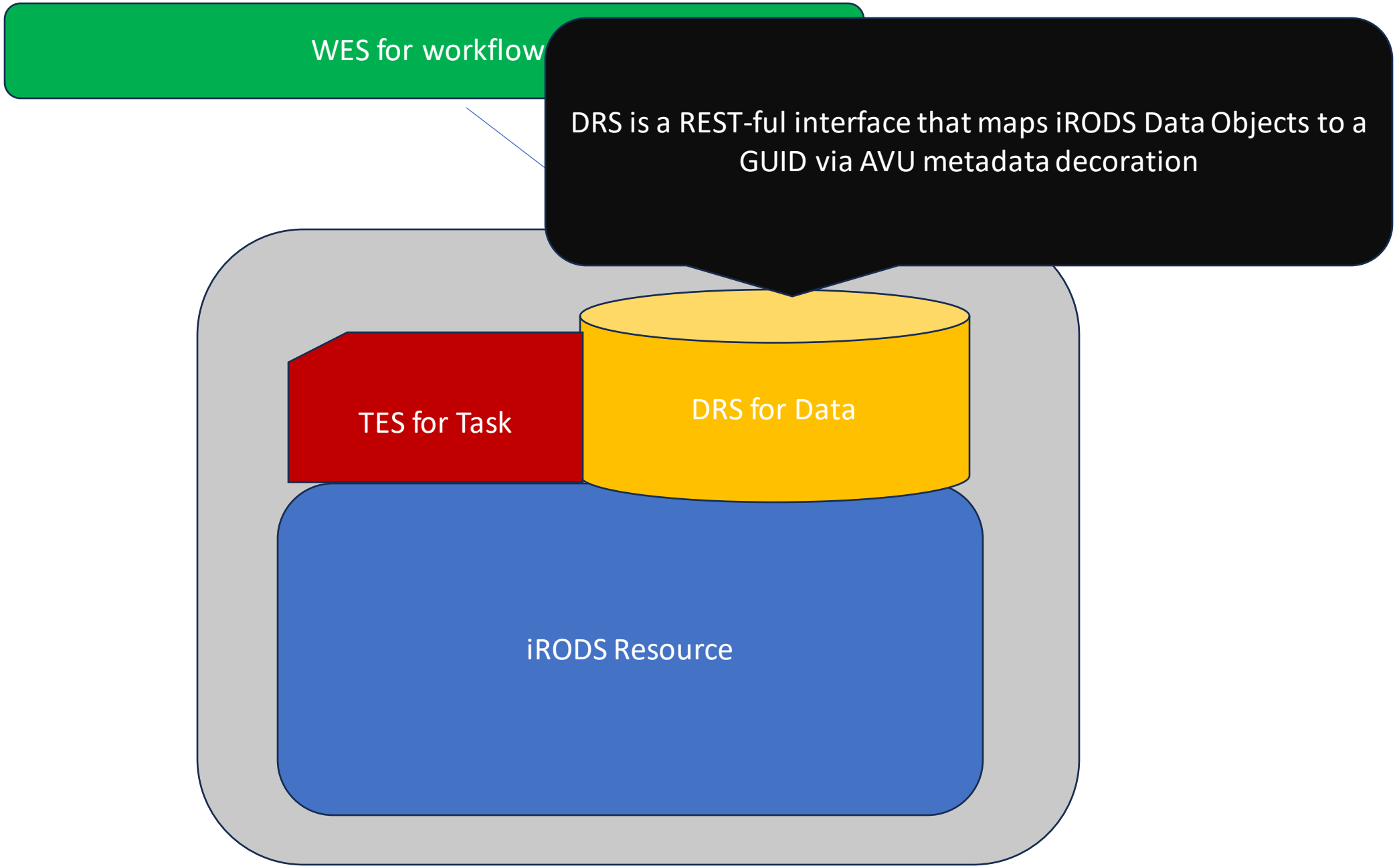
- Registry of Tools
- Assembled into workflows
- Dispatched to task runners
- Referencing Data
- Mediated by data usage policies and researcher identity




WES for workflows
TES for Task
An iRODS Resource is an on-prem analogue of a data set in a particular location (cloud+region) and can take advantage of data locality
iRODS Resource

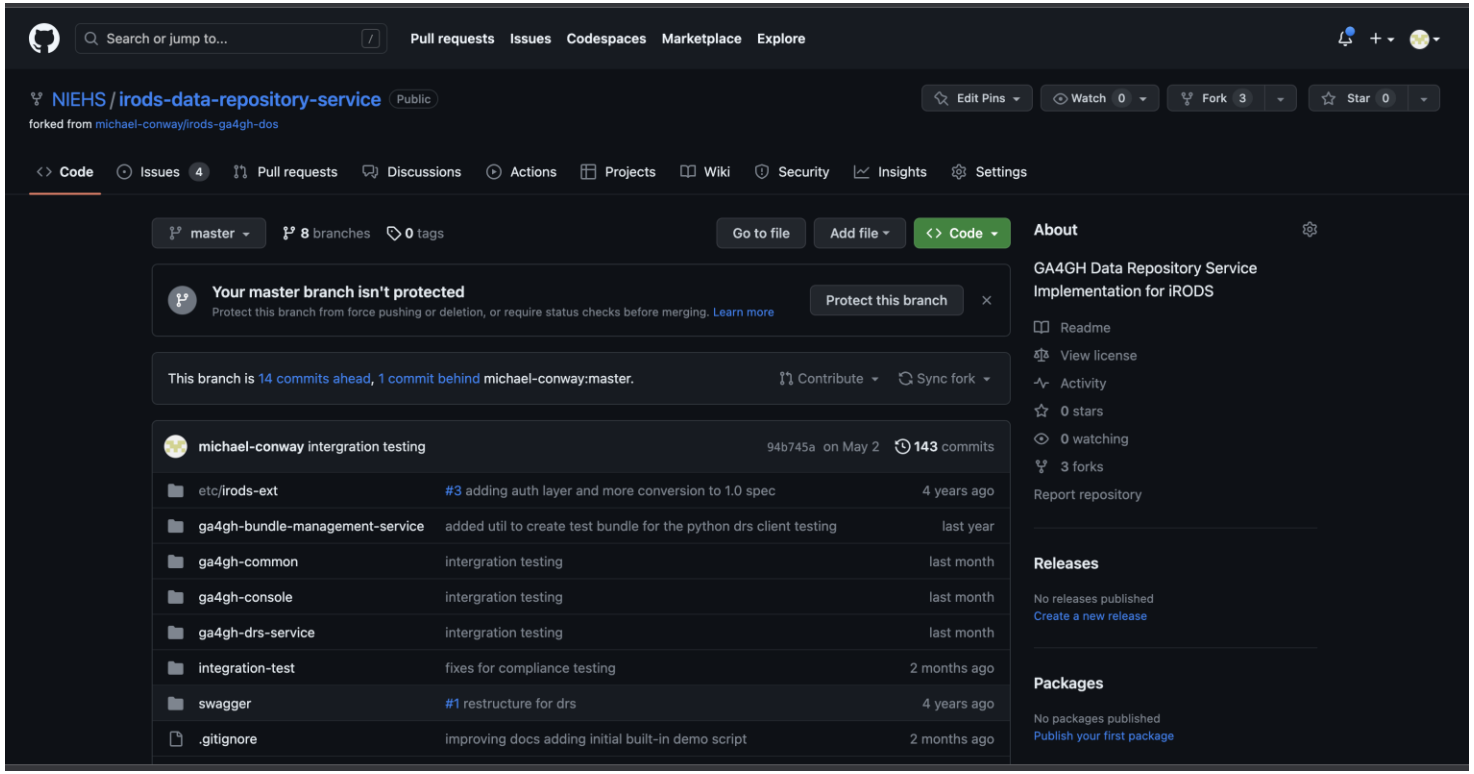

WES for workflows
Descriptions of Data Usage limitations are married with accessor identity/claims - this is a natural application of iRODS Policy-Based Data Managment
TES for Task
DRS for Data
iRODS Resource


WES for workflows
TRS is a task runner with a REST-ful interface that shares some characteristics of the iRODS Rule Engine
TES for Task
DRS for Data
iRODS Resource


WES for workflow
DRS is a REST-ful interface that maps iRODS Data Objects to a GUID via AVU metadata decoration
TES for Task
DRS for Data
iRODS Resource

iRODS DRS Interface

- https://github.com/NIEHS/irods-data-repository-service
- Implements Version 1.2 https://ga4gh.github.io/data-repository-service-schemas/preview/release/drs-1.2.0/docs/
- Currently testing with DRS Compatability Suite (https://github.com/ga4gh/drs-compliance-suite)
- Previously demonstrated at GA4GH Connect, GA4GH DRS Hackathon
- Current work:
  - Adding Authn via Keycloak
  - Upgrading to 1.3 Spec



Firing up the included Compose framework

This starts an iRODS server, the DRS API, as well as a ’starter’ console that emulates potential iCommand interfaces.

```
conwaymc@ALMBP02246093 ~ % docker ps
CONTAINER
ID   IMAGE                                COMMAND             CREATED        STATUS
PORTS                    NAMES
0b717911971d   michaelconway/ga4gh-drs:latest       "/runit.sh"          2
minutes ago   Up 2 minutes   0.0.0.0:8080->8080/tcp          irods-drs
e3cc8967907d   michaelconway/irods-rest2:1.0.1      "/runit.sh"          6
weeks ago     Up 2 minutes   0.0.0.0:8888->8080/tcp          irods-rest
324d035af2d7   michaelconway/ga4gh-console:latest   "/runit.sh"          6
weeks ago     Up 2 minutes                                   ga4gh_console
15aefedb2a2d   compose-irods-catalog-provider       "./start_provider.sh"   6
weeks ago     Up 2 minutes   0.0.0.0:1247->1247/tcp, 1248/tcp   irods-
catalog-provider
conwaymc@
```

GA4GH Console

- Follows iCommands style
- Make test files for testing
- Turn collections into bundles

In reality, making a bundle just adds AVU metadata at collection and data object level with GUIDS and Checksum information

```
shell:>help
AVAILABLE COMMANDS

Built-In Commands
      clear: Clear the shell screen.
      exit, quit: Exit the shell.
      help: Display help about available commands.
      script: Read and execute commands from a file.
      stacktrace: Display the full stacktrace of the last error.

Drs Bundles Command
    * icd: Change working directory in iRODS
      iinit: Initialize connection
    * ilistdrsb: List all DRS bundles
    * ils: List directory contents
    * imakedrsb: Make a DRS bundle at current directory
    * ipwd: Print working directory in iRODS
    * irmdrsb: Remove a DRS bundle by directory path or GUID
      maketestbundle: Create test bundle

Commands marked with (*) are currently unavailable.
Type `help <command>` to learn more.
```

Make a bundle

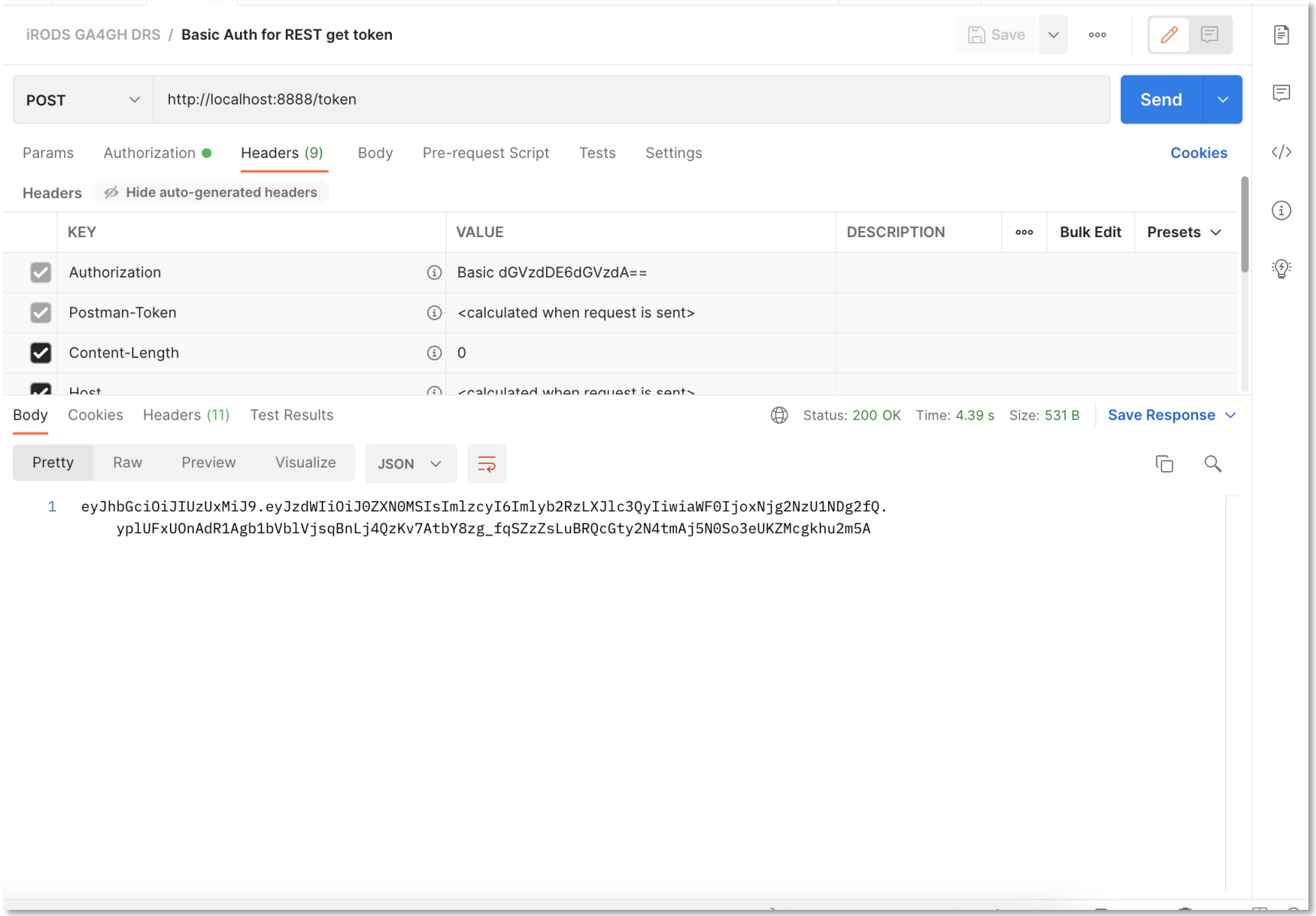
- Mark iRODS collection as a DRS Bundle
- AVUs mark collection and data objects with GUIDs
- Does some checksum computation for the whole bundle and adds as AVU

```
shell:>ils
/tempZone/home/test1
        /tempZone/home/test1/testbundle2
        COLLECTION

shell:>icd testbundle2
/tempZone/home/test1/testbundle2
shell:>imakedrsb
created bundle with GUID:64487235-4bb0-4849-8eff-957581ff933f
shell:>
```

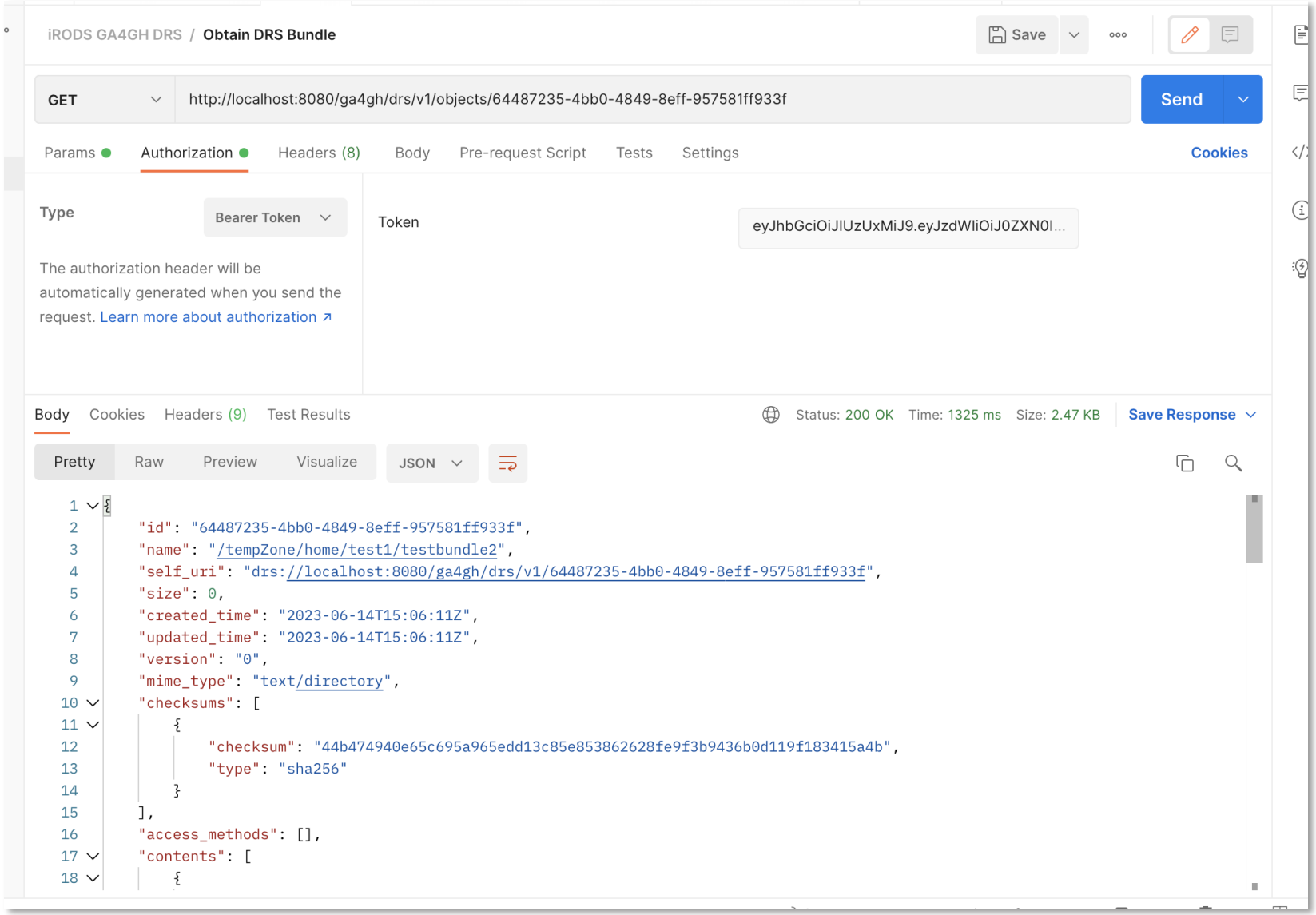
Obtain a Bearer Token (JWT)

- Currently via REST Client
- KeyCloak Implementation is next step!



Obtain information on Bundle

- Pass a GUID
- Describes the bundle and the constituent objects



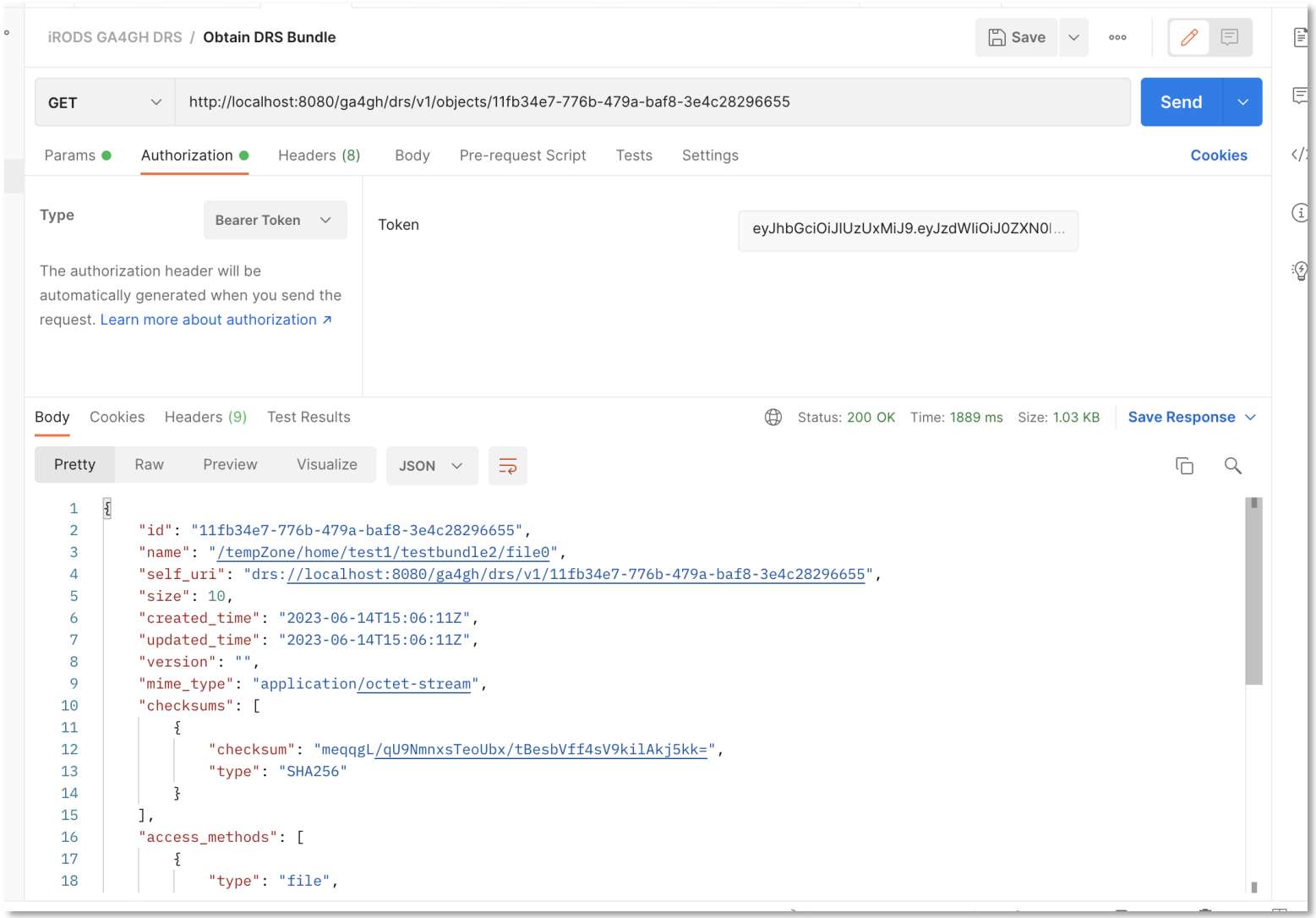
DRS File in Bundle

- Response highlights a DRS Object in the bundle and a URI that references

- "contents": [
- {
- "name": "file0",
- "id": "11fb34e7-776b-479a-baf8-3e4c28296655",
- "drs_uri": [
- "drs://localhost:8080/ga4gh/drs/v1/objects/11fb34e7-776b-479a-baf8-3e4c28296655"
-],
- "contents": []
- },

Use DRS Object ID

- Returns similar structure with some important additions
- Let’s highlight the access methods



Access Methods

- Type is focused on HTTPS as well as S3, here we add an iRODS type but would require special provisioning in the task running environment
- iRODS S3 interface development enables new access methods in DRS
- HTTPS can target the new iRODS REST interface, here it's using the prior Jargon interface for prototyping.
- Region in DRS is focused on cloud but can map to iRODS zone:resource for data locality


```
"access_methods": [
{
    "type": "file",
    "access_url": {
    "url": "irods://test1@irods-catalog-provider:1247/tempZone/home/test1/testbundle2/file0",
    "headers": []
    },
    "access_id": "irods",
    "region": ""
    },
    {
    "type": "https",
    "access_url": null,
    "access_id": "irods-rest",
    "region": null
    }
],
```

Pass DRS GUID and access method to obtain the Access URL

- This step converts the DRS reference into an accessible endpoint
- Invoking this method creates an iRODS REST API call with an attached iRODS Ticket