A year of iRODS: Lessons Learned

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KU Leuven

- Founded in 1425
- Belgium's largest university
- 15 faculties in 10 cities
- ~21000 employees and ~60,000 students
- ~7600 researchers and ~6,200 PhD students
- #1 Reuters Ranking of Most Innovative Universities in Europe 4 years
- #45 in the Times Higher Education World University Ranking (2020)
- #84 in the QS World University Ranking (2021)
The VSC HPC community

Diversity!!!

- Technology: 19%
- Molecular Modelling: 29%
- Physics: 14%
- Astronomy and Astrophysics: 18%
- Life Science: 4%
- Earth Science: 1%
- Computational Science: 1%
- Chemistry: 13%
- Psychology: 3%

- 200 users
- 80 projects
- 300,000 jobs

Scientific domains
Data types
Data sizes
How iRODS fits in here .....
Why an (active) data repository?

Help and encourage users to apply good data management practices

- Give context to data
- Search data
- Automate data workflows
- Share data
- Secure data
- Publish
Pilot users

- **Storage4climate** (Climate change research)
- **CLARIAH-VL** (History research)
- **EXIMIOUS** (Human Exposome)
- **FLANDERS MAKE** (3D printing)
- **VIB** (Biotechnology) – usegalaxy.be
- **VIB-KU Leuven** (ASAP project)
System architecture (pilot environment)

Clients
- YODA
- metalnx
- Cyberduck
- DAVRods
- iCommands
- Python Client
- Go front-end

iRODS
- HA Proxy
- iRODS servers (VM)
- HOST
- MySQL
- Database Cluster
- iCAT
- 1 zone
- All containerized (docker/nomad):
  - 6 iRODS server containers
  - Metalnx containers
  - 2 WebDav containers
  - ...

Storage servers
- iRODS storage servers
- Posix Resc1
- iRODS primary
- Ceph Resc3
- Testing
- DC Heverlee
- 3km
- DC Leuven
- iRODS storage servers
- Posix Resc2
- iRDS Replica Resc1
1 year in numbers

- 50 registered users (20 active)
- 475 TB uploaded
- 55,000 collections
- 6+ million files
- 200 unique metadata attributes
- 200,000 metadata values
- Average file size 180MB
- 3 times data migrated between storage devices
- 300 files lost
Start is hard

- First step is easy (demo setup)
- But ...
  - move from demo to real life is more complicated
  - Learning curve (finding the optimal iRODS way of working)
  - Documentation is not always clear (or is not enough)
  - Need to figure out when and how to create rules inside iRODS to support domain specific use cases
MySQL or not MySQL?

- It is possible (we do!)
- No big performance differences noticed so far (more tests needed)
- But ...
  - MySQL iCAT initial installation needs patches (UTF-8 encoding, ...)
  - Metalnx search does not work
    - See: https://github.com/DICE-UNC/jargon-irods-ext/blob/4a20477a4a4dccb3eb59cf73b7ebdcd6d584d2/emc-metalnx-services/src/main/java/com/emc/metalnx/services/irods/utils/SpecificQueryProviderFactoryImpl.java#L44-L53
  - Issues with atomic metadata
    - Inconsistent use of low level drivers, MySQL conflict (https://github.com/irods/irods/issues/4917)
  - Database schema uses case insensitive VARCHAR columns by default, where the PostgreSQL schema is case sensitive (breaks imeta upper qu ... for example)
  - MySQL transactions behaves different that PostgreSQL transactions
The storage dilemma

- Which storage type is best? Which is the best configuration/storage hierarchy?
  - We have been playing around: xfs, NFS, S3 (Ceph, NetApp Storage Grid), BeeGFS, GPFS

- So far ... 
  - NFS the most stable and performant
  - S3 was unstable and less performant (TBD: test new S3 plugin and Ceph NFS gateway)
  - BeeGFS was less performant
    - ibun did not work – hard links not supported
  - GPFS stable and similar in performance as NFS
  - Replica management is iRODS not yet robust enough (logical lock might help)
  - We have seen memory leaks issues in some storage systems (not yet known why)
iRODS user experience

- CLI/Python works for most HPC users (advanced users)
  - We created user guides and training (incl. hands-on and examples)
  - We developed a PRC extension:
    - to allow to use wildcards
    - Add job information as metadata
- But also needed ...
  - Other direct access to data (NFSRODS, WebDav (Davrods), irodsfs)
  - A user friendly GUI
The GUI wars

YODA
- User friendly
- Implements the whole data life cycle (ingest to publication) -> RDM tool
- Implement full control ACLs and data access
- Implements a rich set of policies (for specific workflows)
- Metadata at collection level and configurable templates (based on DataCite)

Metalnx ...
- User friendly (but sometimes too much options)
- Direct interface to iRODS (no policies)
- Metadata at collection and files level (simple templates possible)
- Search function (so far not for us)
The GUI wars

Although Yoda and Metalnx works well for some use cases

- They do not coexist nicely
- YODA shadow groups broke some Metalnx functions

So ...

- We will stop using YODA
- We will still keep using Metalnx (and try to fix the problems)
- In parallel:
  - We are doing a PoC for an own developed portal
  - We have developed a light front-end (based on the Go Client):
    - Custom authentication based on oauth (while waiting for interactive PAM)
    - Users and group management features
    - https://github.com/cyverse/go-irodsclient
Yet another iRODS portal?

Rationale ....

- Easy to use, domain specific web based interface(s)
- Support a wide range of use cases
- Mix (external) business logic and iRODS rules
- Modular approach, (re-usable) building blocks
- Centrally supported (ICT services, us 😎), possibly extended by end users
- Leverage search engines for discovery, analysis and query scaling
PoC: technology choices

- Python with iRODS Python Client
  - Extended with a home developed higher level API
  - Leverage the many available scientific libraries when appropriate
- Flask (lightweight) web application framework
  - (nested) Blueprints (modularity)
  - Flask-WTF (forms)
  - Waitress/Gunicorn (HTTP server)
- Client side: Vue.js javascript framework
  - Standardised @ KULeuven web teams
- Search engine: OpenSearch (Elasticsearch)
  - Apache Solr as a future option
- Meta-data templates
  - TBD (Yoda/JSON, TWG initiative, RUG, our own ..)
Conclusion

- iRODS is a flexible and powerful tool for data management
- The learning curve is high but the results make it very valuable
- Some additional documentation and how-to could help to find the way to beginners
  - Community curated wiki on best practices, links and more ...
- Some components need to be more tested against other DB than PostgreSQL
  - we will try to contribute to it

- And there is a great, dynamic and fantastic community!
  - Thank you for the help and support!
Next steps

- Finalize design and acquire the production storage infrastructure (min. 6-8PB)
- iRODS features to explore, test, (deploy)
  - Federation
  - NFSRODS
  - Landing zone/automatic ingestion
  - User portal including metadata standards/templates
  - Search engine
  - Globus
  - GDPR (access control, security, auditing, ...
The team (growing)

Paul Borgermans  Mustafa Dikmen  Jef Scheepers  Maxime Van den Bossche  Ingrid Barcena

User Support  User tools  Policies  Documentation

iRODS middleware

Peter Verraedt  Jan Bongers

Tom Vanmierlo  Kristoff Van Buggenhout  Bart Vanneste

Storage
Thank you!