SODAR – THE IRODS-POWERED SYSTEM FOR OMICS DATA ACCESS AND RETRIEVAL

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Background and Goals
Core Unit Bioinformatics (CUBI) at BIH

Consulting

Standardized Data Processing

• Access to tried and tested Omics workflows
• Infrastructure to process large (“inhouse” or “public”) data sets
• FAIR Data Management
• User Empowerment

Scientific Services

• Bioinformatics analysis tailored to specific needs and questions
• Access to Know-How of the Core Unit
• Pet / Research / Technology Development Projects

Training
High Throughput Data from Various Sources

• Sequencing (genomics, transcriptomics..)
• Metabolomics
• Proteomics
• High throughput equals large data sizes and many measurements
• Data is heavily processed and reduced in size
  • Many files are necessary and worth keeping

Traditional Data Management

• Modeling study data in spreadsheets
• Files stored and shared using e.g. portable drives
Omics Data at CUBI

Key Requirements for Sustainable Data Management

• Large scale storage and archival of raw data
• Maintain context between study design meta-data and raw data files
• Data protection and access control
• Adhering to the FAIR principles (*Wilkinson et. al. 2016*)
  • Findable, Accessible, Interoperable, Reuseable
• Multi-institute collaboration
Our Goals

Develop a System for Omics Data Access and Retrieval

- System to aid researchers and project owners manage and access omics data
- Support omics study design modeling
- Managed storage of large scale raw data
- Govern user access to data
- Linking data to third party systems / public data sources
- Enable collaboration between multiple organizations
Why iRODS?

Reasons for Choosing iRODS for Mass Storage

• Scalability and replication support
• Built-in meta-data functionality
• Potential in rule engine for e.g. data validation
• Flexibility: allows integration with out own infrastructure
• PAM support enables multi-organization authorization
• Nice community :)

Why not Go for Cloud?

• Data protection issues
• Cost issues
• iRODS offers better flexibility than “just” object storage
• S3 is there if needed
SODAR Design
SODAR Basics

SODAR for the User
- Web site for user interaction
- REST APIs for programmatic access
- Access with existing institute credentials, supports multiple organizations

Projects and Roles
- Data is organized in projects and categories
- Project-specific roles are assigned to users
- Project meta-data and application data maintained in the SODAR database, certain meta-data also mirrored in iRODS
- Audit trails generated by the system with the ability to log project activity
- ID management: UUIDs generated for each project object, access via UUID
Study Design via Sample Sheets

Sample Sheets for Study Design

- Sample sheets contain sample and process meta-data for project studies
- Modeled in the ISA-Tools standard: https://isa-tools.org/
- Investigation > Study > Assay
- Graph models commonly represented as tables
- SODAR features a built-in browser to view and search the sample sheets
- Links out to raw data and external tools from e.g. specific samples
- CUBI altamISA parser used to read and write ISA model files (GitHub: bihealth/altamisa)
Data Files in iRODS

- Files organized in collections by project
- User access managed by SODAR
- Access via the same pre-existing institute credentials
- Links to iRODS resources provided in the web UI

Data Uploads via Landing Zones

- Files in project repositories are read-only
- Upload through user-specific landing zones
- Data validation → Rules for accepting data into repository
Managing iRODS Transactions

SODAR Taskflow: an In-House Transaction Engine

- Handles automated validation and moving of landing zone data into project repository within iRODS
- Reverts the transaction if failures are encountered → user can go back to alter their data in the landing zone
- Locks each project during transactions, to prevent data corruption
- REST API based Python service, uses Openstack Taskflow
- Updates transaction status in the SODAR web interface via its API
- Also makes use of iRODS rules (to be expanded in the future)
Accessing iRODS Data

Davrods
- DAV mounting
- Web-based file browsing
- Random access to large files

Integrative Genomics Viewer (IGV)
- Automated session file generation and serving
- Generated from sample sheets by SODAR, linking to iRODS files via Davrods

iCommands
- Working in landing zones also possible for command line and scripts
Core Features as a Separate Project

• Project management & UI framework
• Reusable project apps
• Ability to create and install new apps in a plugin fashion
• Can be used to build new sites with their own configuration, applications and functionality
• Allows sharing project access between multiple sites
• Python package containing installable Django apps and an example site

Availability

• Publicly available In GitHub: bihealth/sodar_core
• Latest release: v0.6.2 (2019-06-21)
SODAR Technology

Web UIs and Applications
- Python 3
- Django
- Bootstrap
- Font Awesome
- JQuery
- Vue.js
- Ag-Grid
- Node/Webpack

Back-End and iRODS
- Davrods
- Python-Irodsclient
- AltamISA (ISA-Tools parser developed in CUBI)
- OpenStack Taskflow & Tooz
- Celery
- PostgreSQL
- Redis
SODAR Architecture
Rare Disease Genomics Use Case Demonstration
Status and Ongoing Work
Status and Ongoing Work

SODAR Usage
- Deployed at CUBI in beta
- Second instance in use at Uni. Bonn
- Actively used in dozens of projects with collaborators
- Talks with other organizations interested in adopting SODAR

SODAR Development
- Source code will be published, as well as submitting scientific publications
- SODAR Core already made public on GitHub
- SODAR Core in use as the platform for several other CUBI software projects (Varfish, Digestiflow..)
- Development is ongoing

Ongoing and Future Work
- Integrated editor for sample sheets
- More advanced validation of data in iRODS
- A more comprehensive REST API
- Etc., etc.
Conclusions
Conclusions

**SODAR**
- Has proven to be a valuable aid to researchers in CUBI omics projects
- Interest from several organizations
- Core parts also in active use by several other systems
- SODAR and its parts are expected to evolve further

**iRODS in SODAR**
- iRODS was our choice when starting to build initial prototypes
- Remains as the mass storage platform of choice
- Utilized comprehensively from iCommands to Python APIs and Davrods
- We envision more use for e.g. the rule engine in the future
- Deployment to be scaled up in the future as well
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THANK YOU!
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