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

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iRODS User Group Meeting, Utrecht (2019-06-26)

MDC MAX DELBRÜCK CENTER FOR MOLECULAR MEDICINE IN THE HELMHOLTZ ASSOCIATION

CHARITÉ UNIVERSITÄTSMEDIZIN BERLIN

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CONTENT

1. Background and Goals
2. SODAR Design
3. Rare Disease Genomics Use Case Demonstration
4. Status and Ongoing Work
5. Conclusions

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Background and Goals

Core Unit Bioinformatics (CUBI) at BIH

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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

Omics Data at CUBI

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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

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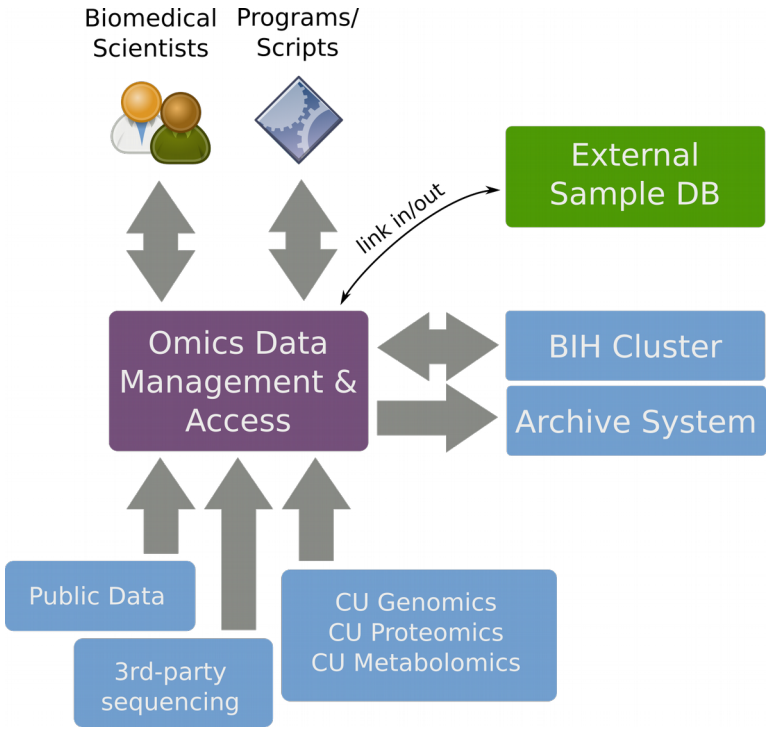
Key Requirements for Sustainable Data Management

- 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)*
    - **F**indable, **A**ccessible, **I**nteroperable, **R**euseable
- 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?

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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

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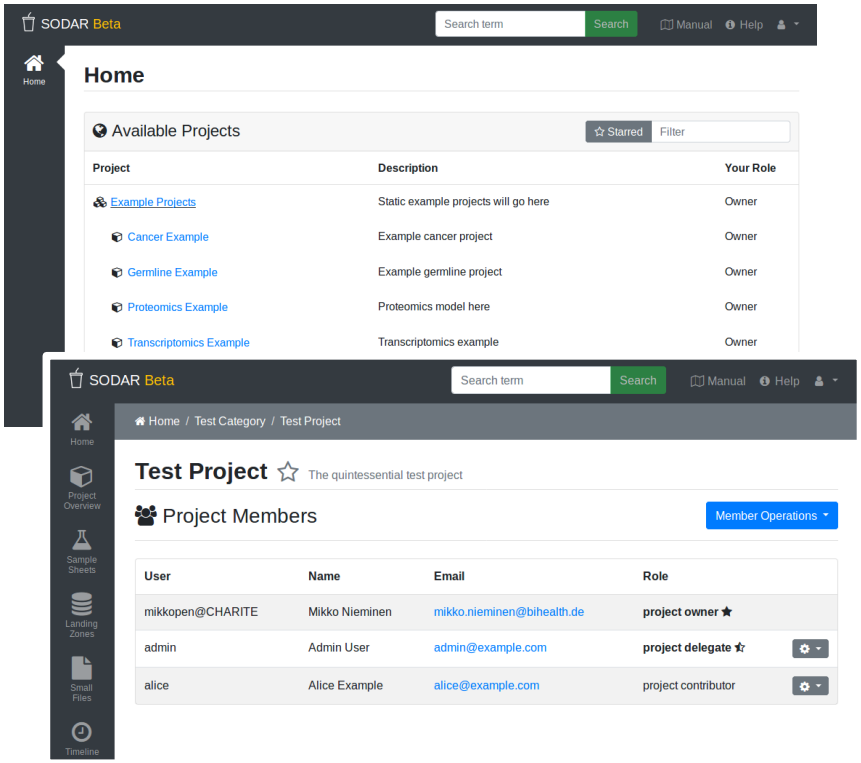
SODAR Design

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

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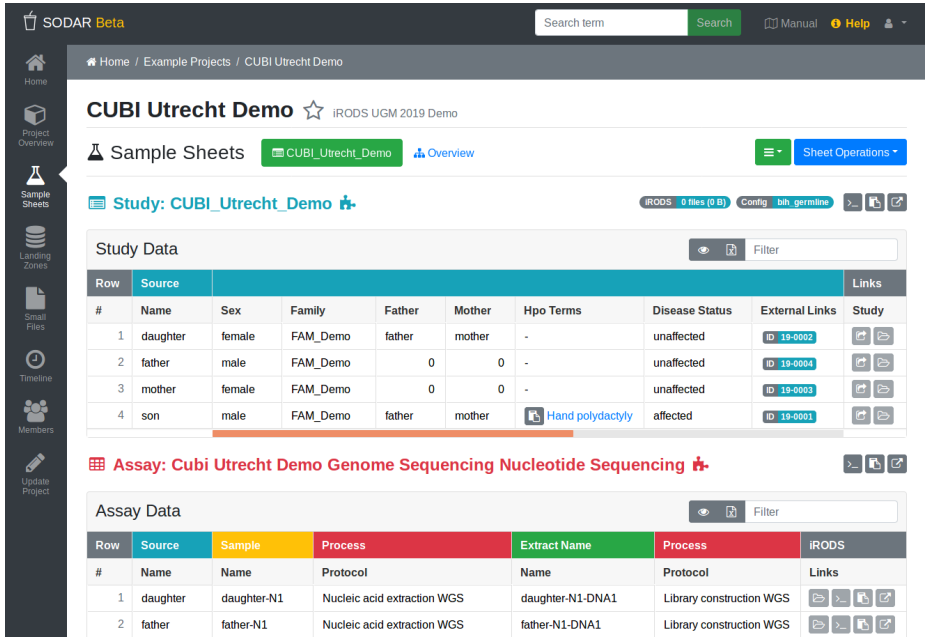

Sample Sheets for Study Design

- 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 File Management in iRODS

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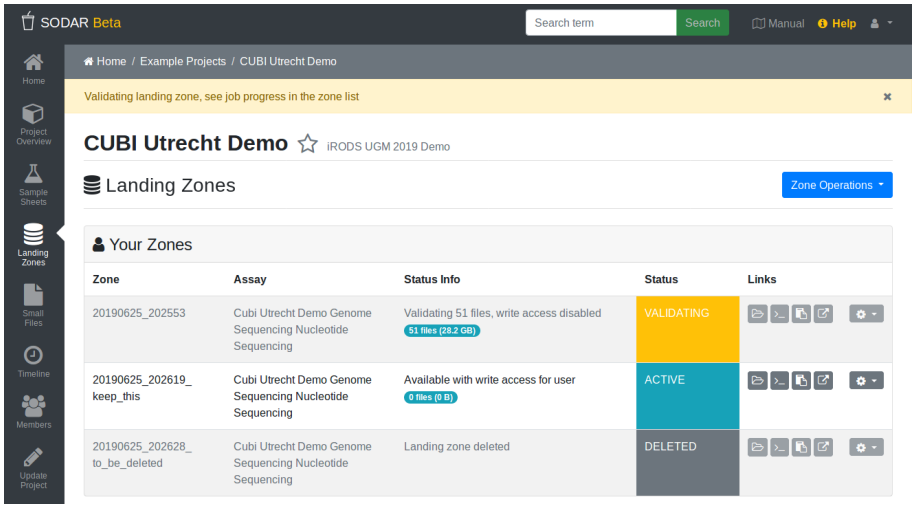


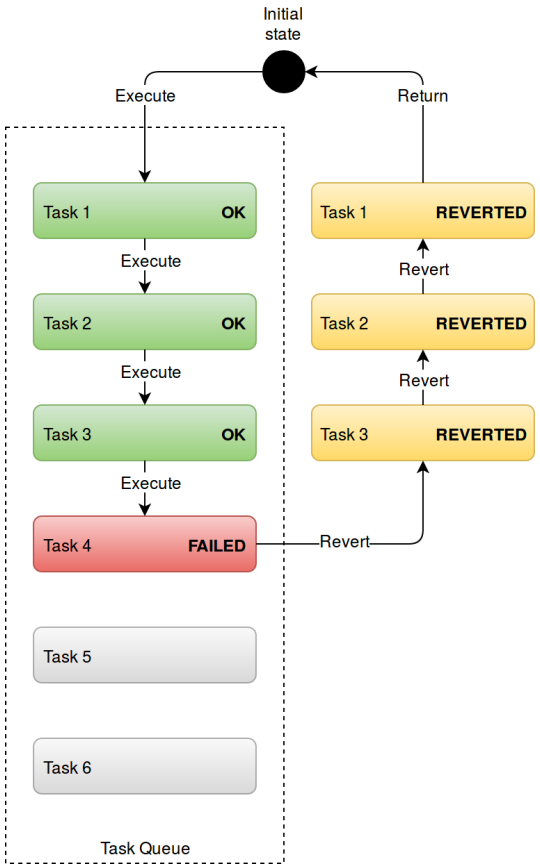
Data Files in iRODS

- 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

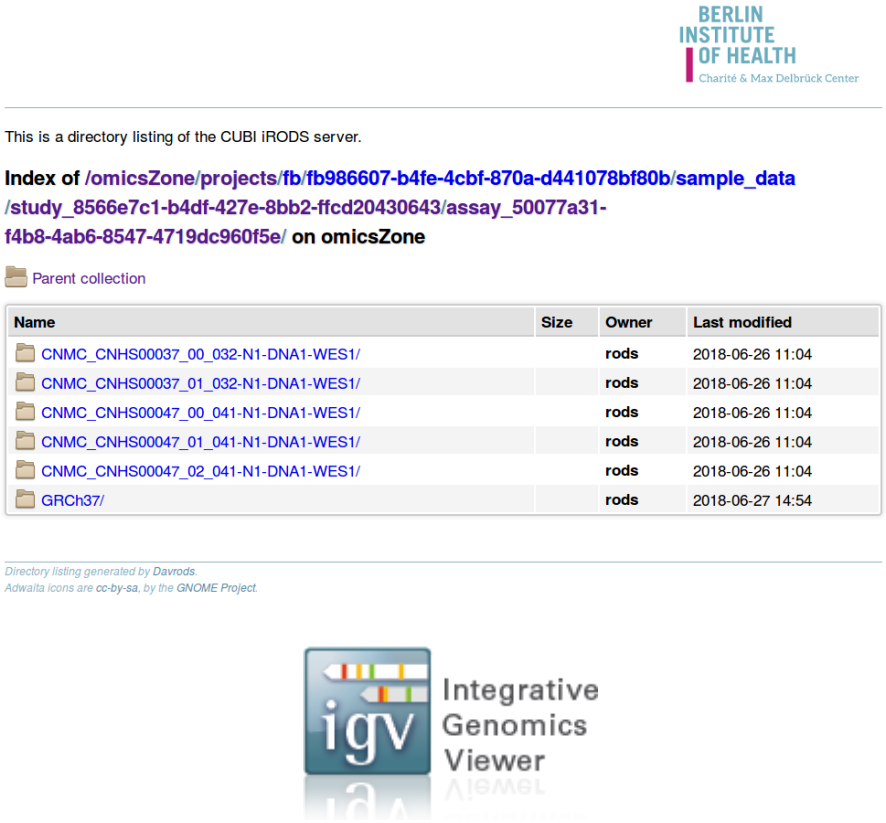
Managing iRODS Transactions



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 co 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

SODAR Core

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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

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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

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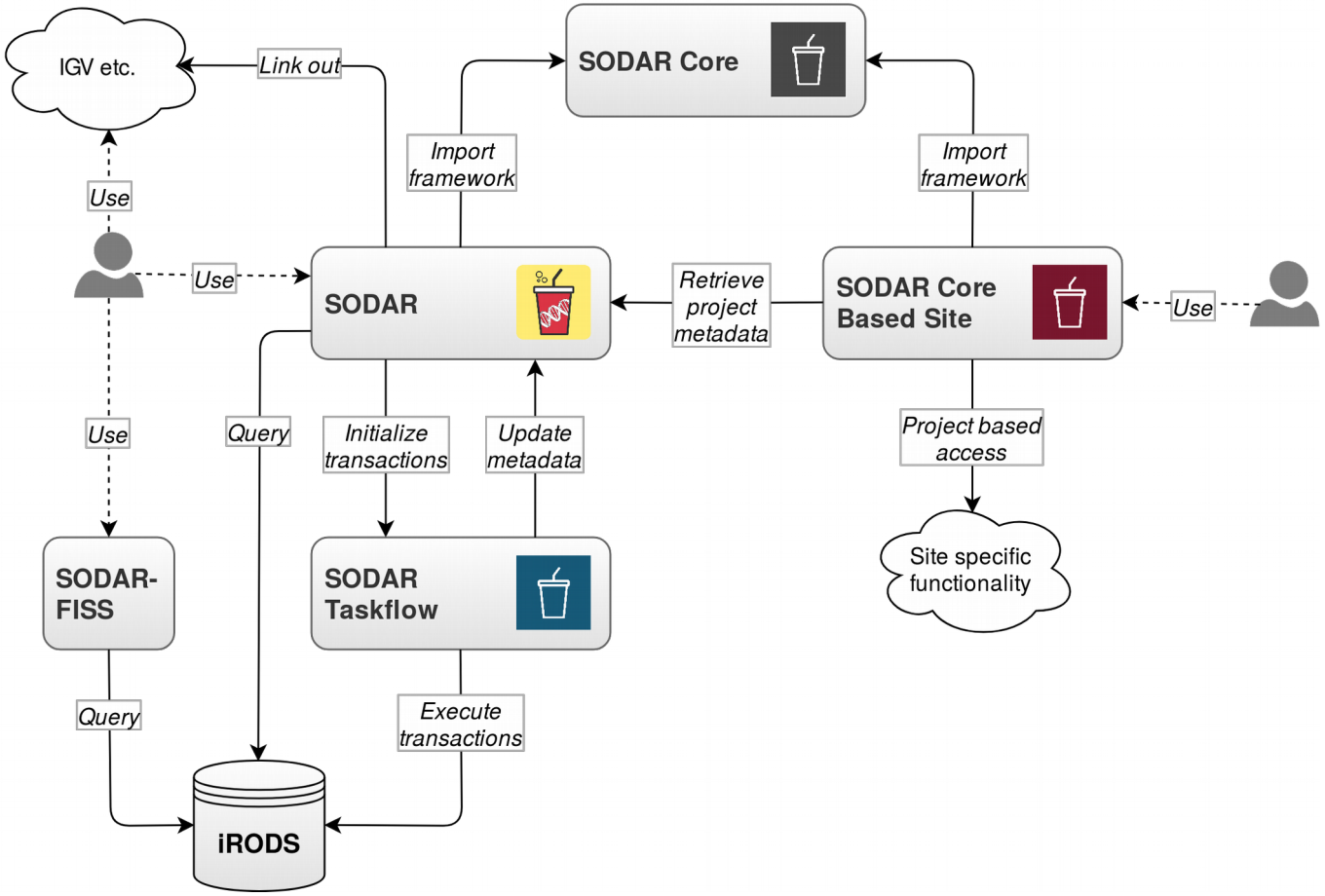

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Rare Disease Genomics Use Case Demonstration

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Status and Ongoing Work

Status and Ongoing Work

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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.

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Conclusions

Conclusions

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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

Acknowledgements

Collaboration

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- Numerous BIH researchers and collaborators using the system, reporting bugs etc.

CUBI

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THANK YOU!

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