Achieving reproducible data workflows: Lightweight tools for safe and efficient data management

C Garbers[1], M Sonntag[1], A. Koutsou[1], C J Kellner[1], J Grewe[2], T Wachtler[1]

[1]Ludwig-Maximilians-Univität München, Germany; [2]Eberhard Karls Universität Tübingen, Germany

Maintaining reproducible data workflows while keeping data in sync, backed up, and easily accessible from within and outside the lab is a key challenge in research. To minimize time and effort scientists have to spend on these tasks, we provide a suite of tools designed for comprehensive and versioned management of scientific data including convenient storage of data, analysis and metadata annotation for easy reproducability, data sharing and re-usability.

Collect and manage all information about your experiment

Main features
- Open metadata format [1]
- Flexible hierarchical key-value storage
- Save to common structured formats: XML, JSON, YAML
- Template system for reusable metadata structures
- Terminology repository [2] for reusable definitions

Graphical user interfaces
- odml-ui [3]: browsing and template editing
- odml-tables [4]: filtering and tabular export
- Available for macOS and Linux

Export to RDF retaining your own terms
- Query metadata using semantic web technologies
- Search cross document via SPARQL queries

Manage data and metadata in one open, versatile format

Main features
- Open data format
- Store data, analysis results, and metadata conveniently in the same file
- Descriptive associations between data, analysis results, and metadata

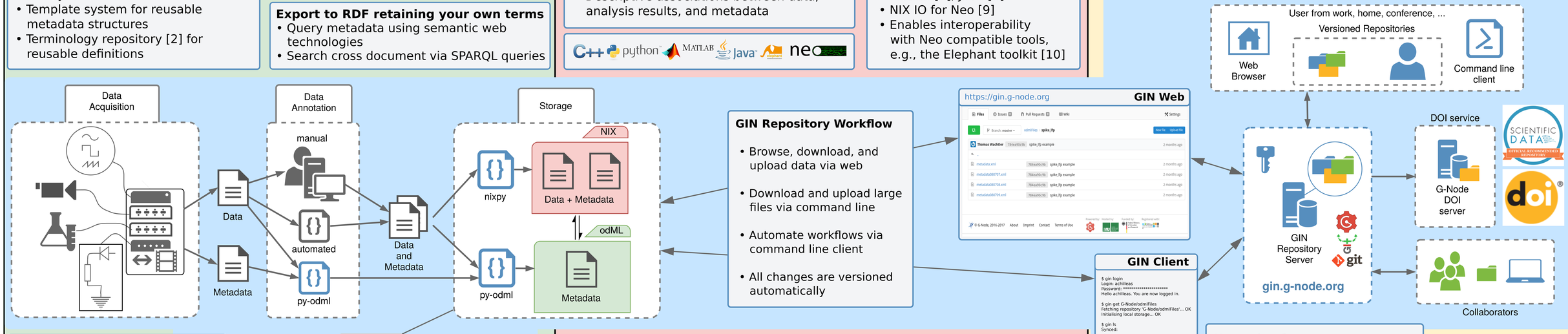
C++ python MATLAB Java neo

- Free open source libraries for multiple programming languages: C++ [5], Python [6], Matlab [7], Java [8]
- NIX IO for Neo [9]
- Enables interoperability with Neo compatible tools, e.g., the Elephant toolkit [10]

Store data securely; publish and collaborate with ease

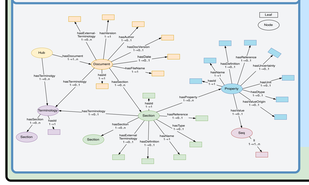
Main features
- Access data from any location
- Free storage for scientific data [12]
- Built in versioning (built on git [13])

- Platform independent
- Secure access
- Public and private repositories
- Citable data by DOIs

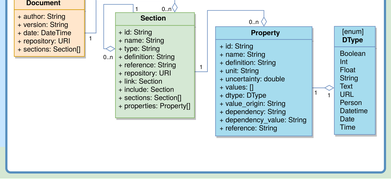


meta.g-node.org
- access diverse metadata datasets
- all datasets are publicly available
- searchable by SPARQL via API and web

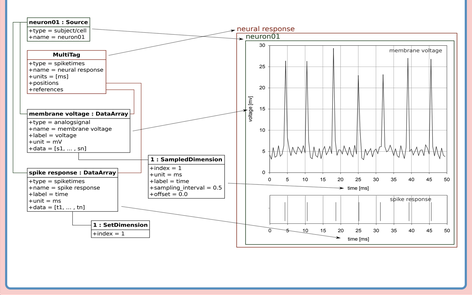
odML RDF schema



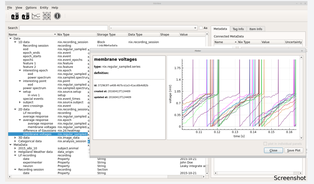
The odML Metadata format



NIX usage example



NixView GUI [11]



- Windows, macOS and Linux
- Convenient exploration of data and metadata of NIX files
- Browse raw data via tabular display and export to CSV
- Built in plotting and figure export

Upcoming features
- Format validation
  - BIDS, odML, NIX, custom formats
- CI for scientific data: automated tests for scripts and data integrity
- automated export of odML to RDF

Collaboration
- User management
- User Access Levels
- On and offsite collaboration

Resources

[1] Grewe et al (2011), doi:10.3389/fninf.2011.00016
[2] http://www.g-node.org/projects/odml/terminologies
[3] https://github.com/G-Node/odml-ui
[4] https://github.com/INM-6/python-odmltables
[5] https://github.com/G-Node/nix
[6] https://github.com/G-Node/nixpy
[7] https://github.com/G-Node/nix-mx
[8] https://github.com/G-Node/nix-java
[9] http://neuralensemble.org/neo
[10] http://neuralensemble.org/elephant
[11] http://bendalab.github.io/NixView
[12] https://gin.g-node.org
[13] https://git-scm.com

Contact: dev@g-node.org

Supported by BMBF grants 01GQ1302, 01GQ1509

Federal Ministry of Education and Research