Research Data Management for Computational Science

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and

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Data requirements

- Data produced by scientific software should be recomputable and reproducible.
- This requires:
  - the software itself (with info about the specific version used)
  - raw data (input and output files)
  - provenance metadata
- We need a way of publishing this data and software at the push of a button...
- ...and a way of referencing it correctly in papers.

Online repositories

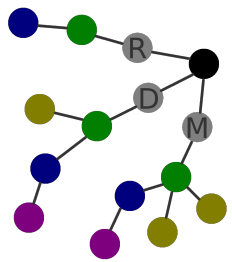
- Organisations such as Figshare (`figshare.com`) and Zenodo (`zenodo.org`) provide hosting for code and datasets.
- Each code/dataset is given its own Digital Object Identifier (DOI).
- Programs developed by users can interface with Figshare and Zenodo via their APIs.

Aims

- Develop a software tool which facilitates the automated publication of both software and data to Figshare, Zenodo and DSpace repositories.
- Incorporate this tool into the workflow of Fluidity – an open-source CFD code for fluid flow simulations (`http://fluidity-project.org`).
- DOIs are 'minted' automatically, and added to the current metadata of simulation output.

PyRDM

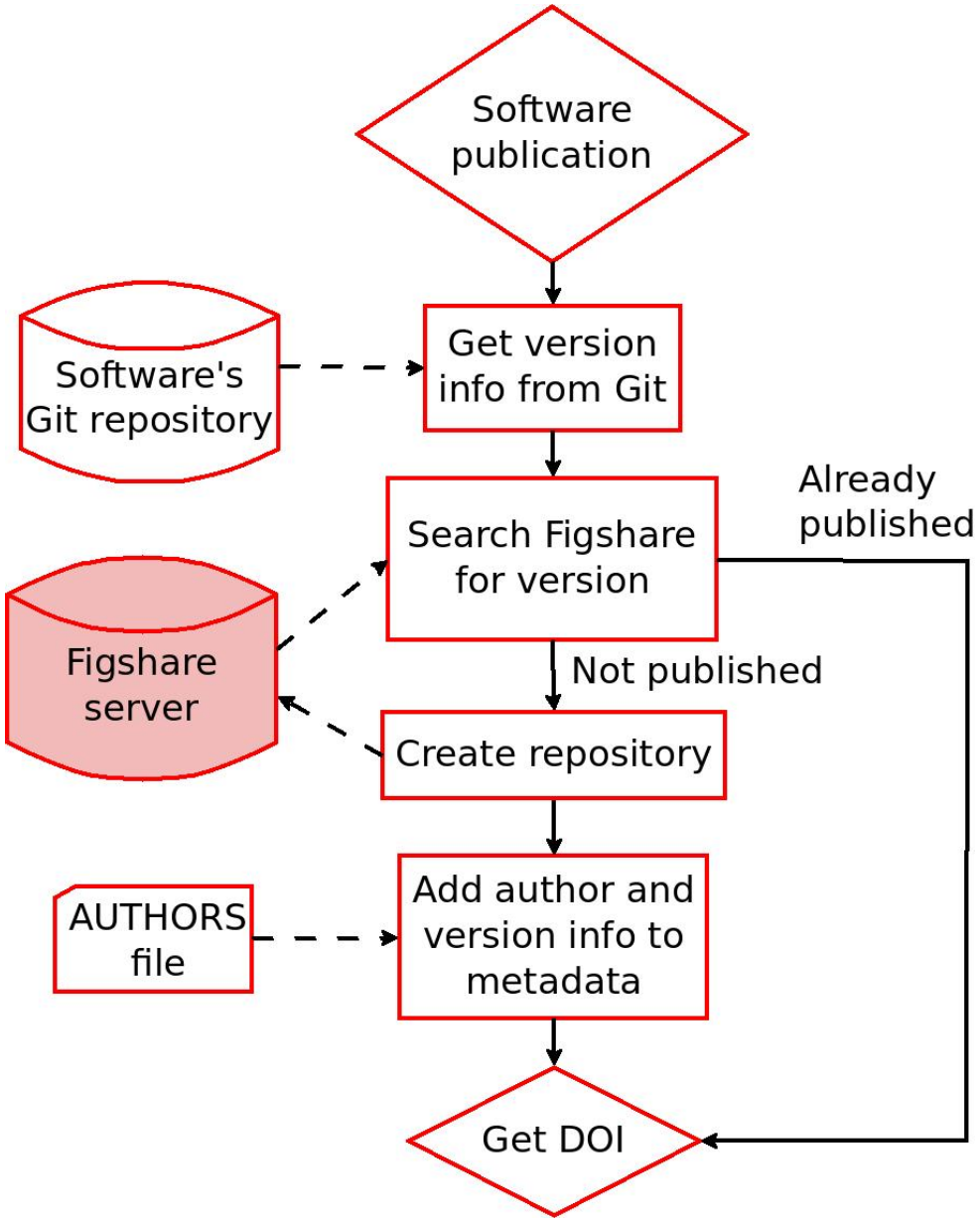
- PyRDM: **R**esearch **D**ata **M**anagement with **Py**thon
- Released under the GNU GPL version 3 license.
- Source code on GitHub: `http://github.com/pyrdm`



- Paper: C. T. Jacobs, A. Avdis, G. J. Gorman, and M. D. Piggott (2014). PyRDM: A Python-based library for automating the management and online publication of scientific software and data. Journal of Open Research Software, 2(1):e28, DOI: `10.5334/jors.bj`

PyRDM

Publishing software source code



PyRDM

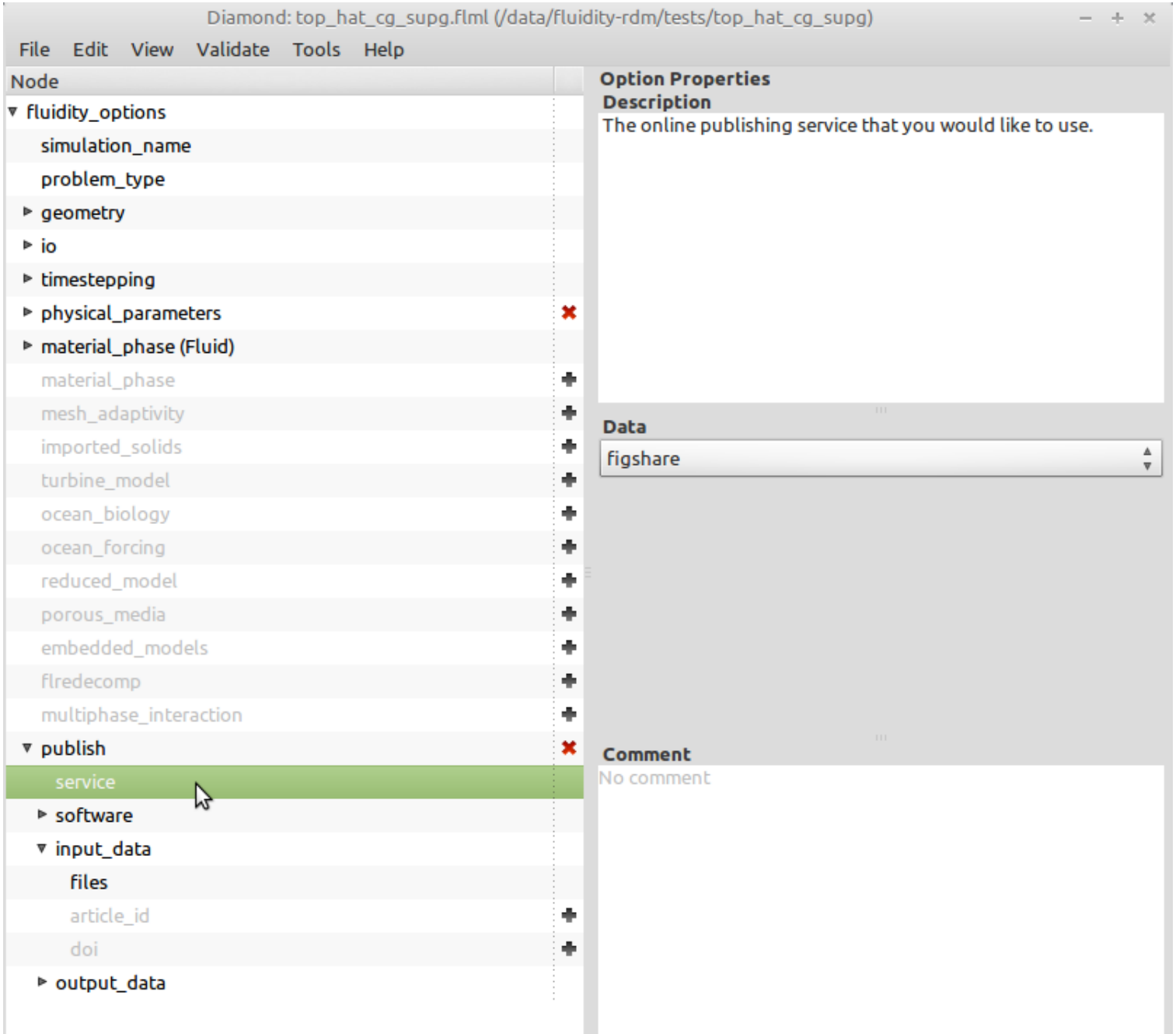
Publishing data

- User specifies data files to be uploaded (e.g. `[*.vtu]`).
- If a new version of the repository is created (e.g. during peer review), MD5 checksums used to selectively re-upload only those files that have been modified.

Application: Fluidity + PyRDM

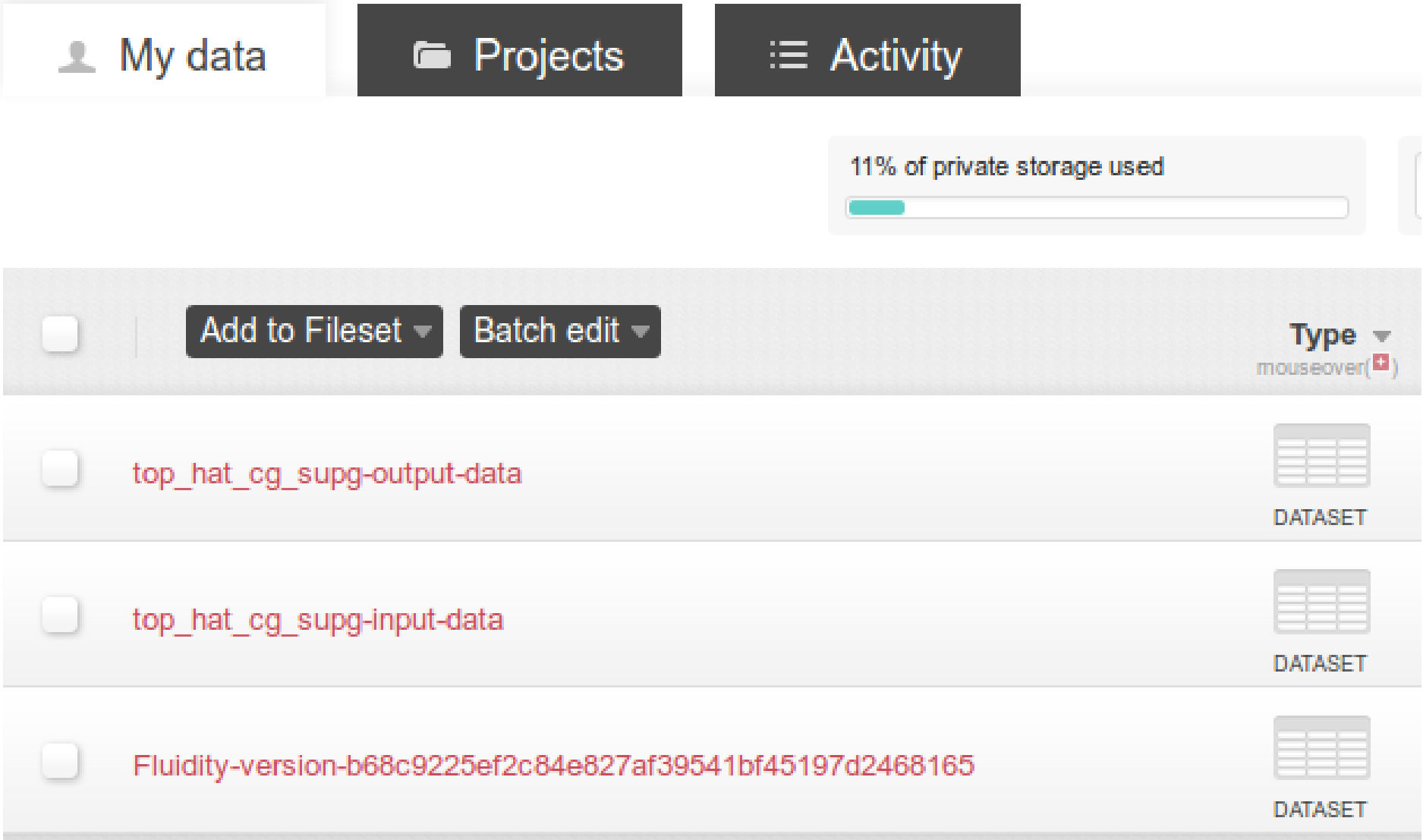
- PyRDM has been integrated into the workflow of Fluidity.
- Users enable a 'publish' option in their simulation's setup file, then run a Fluidity-specific publishing tool which uses the PyRDM library.
- The end-user just has to provide:
  - Their Figshare authentication details.
  - A list of any data files they want to publish (e.g. `*.vtu`).
  - Optionally: an existing Figshare publication ID and DOI.
- DOIs are recorded in the simulation setup file – if the simulation is run again, the same DOI is used to store the data.
- The DOIs for the software and input data are appended to the simulation output for data provenance.

Application: Fluidity + PyRDM



Application: Fluidity + PyRDM

Example: simulation of the `top_hat_cg_supg` test case



Screenshot of software, input data and output data automatically pushed to Figshare.

Application: Fluidity + PyRDM

Example: simulation of the top_hat_cg_supg test case

```
<constant name="FluidityVersion" type="string"
value="1baf80aac1e7e735b1cf182bc20761a0c6df7767"/>

<constant name="SoftwareDOI" type="string"
value="http://dx.doi.org/10.6084/m9.figshare.1035081"/>

<constant name="InputDataDOI" type="string"
value="http://dx.doi.org/10.6084/m9.figshare.1035083"/>

<constant name="CompileTime" type="string" value="May 23
2014 15:22:23"/>

<constant name="StartTime" type="string" value="20140523
154857.775+0100"/>
```

Issues

- Need a better way of affiliating authors - ORCID IDs?
- Lack of API support.
- Need more storage space for private data.