Data Management and Machine-Actionable Reproducibility for HPC

NEC User Group Meeting, Osaka, Japan

2025-05-14 // Andreas Knüpfer, Timothy J. Callow

CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

www.casus.science

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TECHNISCHE UNIVERSITÄT DRESDEN
CBG Max Planck Institute of Molecular Cell Biology and Genetics
HELMHOLTZ CENTRE FOR ENVIRONMENTAL RESEARCH – UFZ
Uniwersytet Wrocławski

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Contents

Center for Advanced Systems Understanding (CASUS)

CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

- Started 2019 in Görlitz / Saxony
- Founded by 5 partner organizations

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Center for Advanced Systems Understanding (CASUS)

- CASUS hosts no large research equipment like most Helmholtz institutes
- … not even the big computing clusters (for good reasons)
- Diverse topics, from biology/ecology to high energy physics and astronomy

Science icons created by Freepik - Flaticon, https://www.flaticon.com

- Computational Science is the connecting element

CASUS combines domain expertise and method expertise

- There are groups with application research in their names
- … and some with methods like "Machine Learning" or "Mathematical"
- And there is Scientific Computing Core (SCC) for Computational Science

Research Data Version Control

Research Data Version Control: Motivation

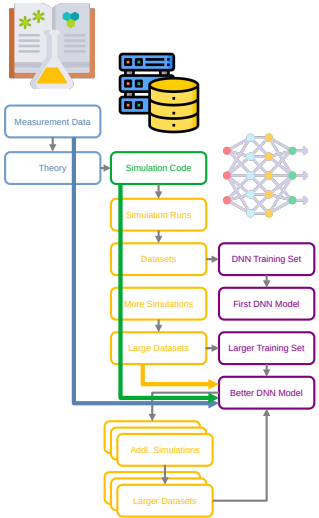
DNN surrogate models from HPC simulation results

- Extensive simulation runs with HPC over months
- … produce labeled data for DNN training

- Start first DNN training with available data early
- … determine feasibility
- … hyperparameter optimization
- … find out how much training data needed

- Iterate for several DNN versions and flavors
- Spot spurious error in some data $\mapsto$ fix in code $\mapsto$ re-run some simulations $\mapsto$ replace affected data

- Which DNN version was trained with which exact subset of the data? Affected by faulty data points?
- Exact versions of the simulation code or the DNN training script used? Track git commit id!



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https://www.flaticon.com/free-icon/database-storage_2906274
https://www.flaticon.com/free-icon/deep-learning_8637092

… we solved it for Software Versioning

- well established and most well known
- Clear steps: commit, push/pull, merge, …
- Command line + GUI + IDE integrations
- **But git is not good for binary data or very large files**

- Central repositories and web GUI
- Authentication and authorization
- Several alternatives like github, Gogs, Gitea, Gin, …

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- Central repositories and web GUI
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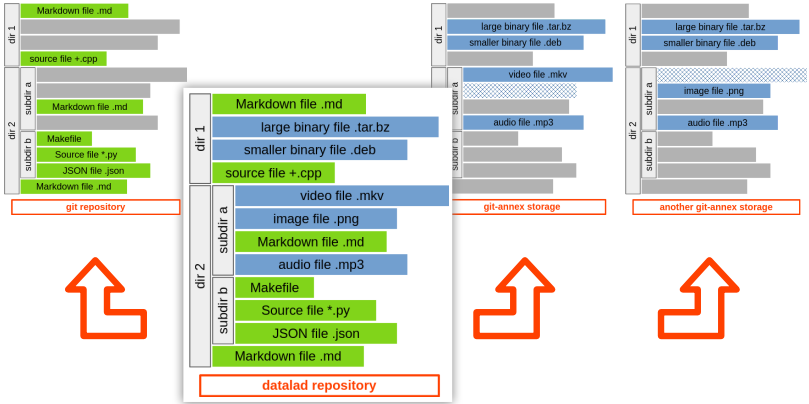
- Several alternatives like github, Gogs, Gitea, Gin, …

- git plugin `git annex`
- new sub-commands
- Manage large binary files via git, yet don't store them in git
- Special git-annex storages instead
- Works with usual sub-commands, GUIs, IDEs, …

git-annex: git for large / binary data

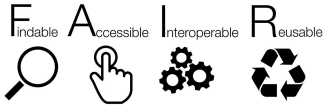
git + git-annex: Text files and binary files go to separate storages:



The F.A.I.R. Criteria and Versioning

- Data versioning is **not** part of the F.A.I.R. criteria
  - Forgotten when they were designed in 2014?
  - Or considered too much to ask?
- Rather few publications dare to ask for fully fledged version control for research data
- Dataset publication with version numbers as the best state-of-the-art approach?
  - Make few data publications, once per year +/-
  - Large sets of archive files (all or nothing)
  - Redundant data between versions, errata lists [a]
- Dataset publication as appendix to papers
  - One point in time per paper
  - Redundant data for successive papers

[a] `https://abcdstudy.org/scientists/data-sharing-archive/`



SangyaPundir, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=53414062

- F1. Unique and persistent identifier
- F2. Rich metadata
- F3. Metadata include the identifier
- F4. (Meta)data searchable

- A1. (Meta)data retrievable by identifier via standardised protocol
- A2. Metadata accessible, even when data no longer available

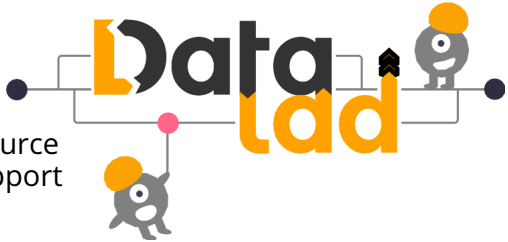
- I1. Formal, accessible, shared, and broadly applicable language
- I2. (Meta)data use FAIR vocabularies
- I3. Qualified references to other (meta)data

- R1.1. Data usage license
- R1.2. Detailed provenance
- R1.3. Meet domain-relevant community standards

Machine-Actionable Reproducibility with DataLad

Machine-Actionable Reproducibility with DataLad

- Distributed data management[1]
- On top of git and git-annex
- Academic background, free and Open Source
- Active community provides hints and support
- simplifies some tasks
- additional functionality



[1] `https://helmholtz.software/software/datalad`, `https://handbook.datalad.org`

Machine-Actionable Reproducibility with `datalad run` and `rerun`

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Record processing steps:

- Use `datalad run` to execute scripts or binaries, preferably with scripts or code sources also in the repository
- Specify input and output files, preferably all part of repository
- See also `datalad containers-run`

```
$>datalad run -m "Resize image" \
  --input git_commit_2x.png \
  --output git_commit_2x.small.png \
  "convert {inputs} -geometry \
   439x439 {outputs}"
```

```
knue@fwu082:~/data/datalad-demo/images > git log -1
commit 4f7a1e6d301e3bdd03aeb6c9e355fb5f2ceb9a23 (HEAD -> mas
Author: Andreas Knüpfer <knue@posteo.de>
Date:   Fri Jul 5 13:19:01 2024 +0200

    [DATALAD RUNCMD] Resize image

    === Do not change lines below ===
    {
     "chain": [],
     "cmd": "convert {inputs} -geometry 439x439 {outputs}",
     "dsid": "be528a88-4333-49cf-9705-0be6e3f84a23",
     "exit": 0,
     "extra_inputs": [],
     "inputs": [
      "git_commit_2x.png"
     ],
     "outputs": [
      "git_commit_2x.small.png"
     ],
     "pwd": "images"
    }
    ^^^ Do not change lines above ^^^
```

Machine-Actionable Reproducibility with `datalad run` and `rerun`

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Work with existing Datalad repository:

- Clone the repository
- All text files get downloaded but annexed files not yet

Get selected / all annexed files: `$> datalad get ...`

Reproduce processing steps: `$> datalad rerun <git commit id>`

- Previous example: `$> datalad rerun 4f7a1e6d`
- Execute same command again, commit results if something changed
- Run with current versions of input files and scripts / binaries
- If necessary do `datalad get` for input files first

- **Added value** when doing all steps the DataLad way

Challenges on HPC and how we solved it

Challenges on HPC

The DataLad reproducibility scheme is very much incompatible with HPC :-(

1. A git repository must not be accessed concurrently: **critical conflict!**
   - Changing files inside in parallel is fine, concurrent git commands are not
2. All `git` / `datalad` calls would be sequential inside the Slurm job
3. Slurm job script not a good reproducibility record if `datalad` commands inside
   - … would need to change `datalad run` to `datalad rerun`

The state of the art workaround: separate clone per job [1]

- For all potentially concurrent jobs in the same repository
- Not necessarily all large / binary files in every clone
- … but all small git bookkeeping files – would your parallel file system like it?

It would not be accepted in the HPC community and by the HPC centers

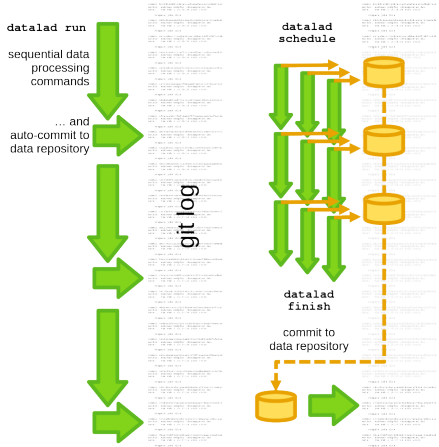
[1] Adina S. Wagner et al. “FAIRly big: A framework for computationally reproducible processing of large-scale data”. In: Scientific data 9.1 (2022), p. 80.

Solution: The DataLad extension for Slurm

DataLad commands around Slurm jobs:

1. Prepare and submit jobs
   - Get annexed files if needed
   - Submit job to Slurm, don't wait
   - New `datalad slurm-schedule` command
2. Finalize jobs and commit of result files
   - After job(s) finished
   - Check and commit files to repository
   - New `datalad slurm-finish` command
3. Re-run jobs
   - `datalad slurm-reschedule <commit-id>`

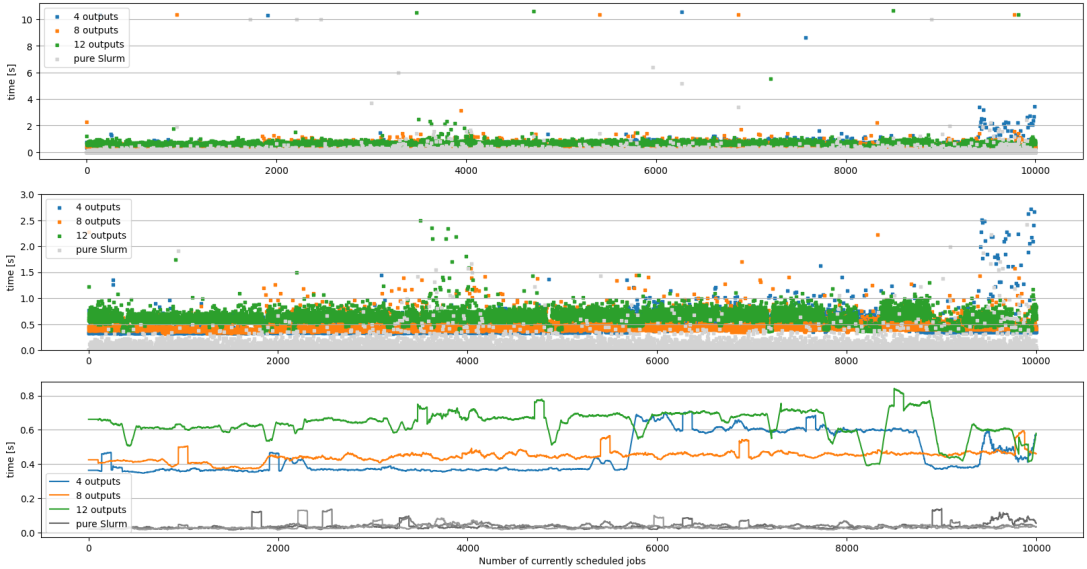
- Call DataLad commands sequentially
- Jobs can run concurrently
- Slurm job script untouched



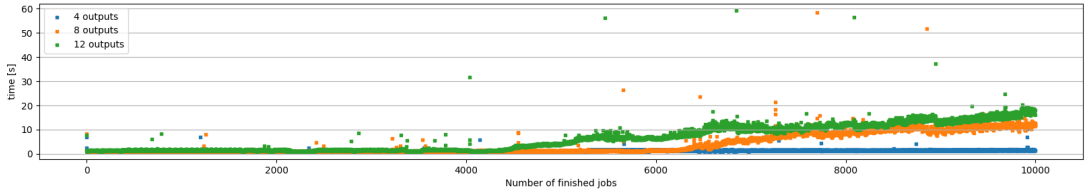
Evaluation

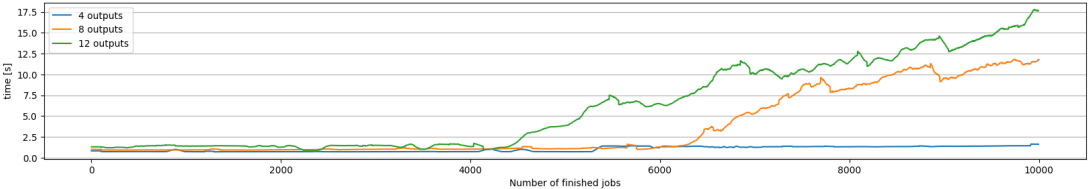
- Evaluation runs with large repositories (number of files)
- Compare to pure Slurm cases

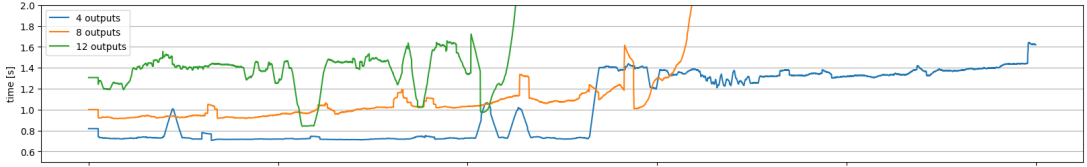
Evaluation: datalad slurm-schedule



Evaluation: datalad slurm-finish







Evaluation Results

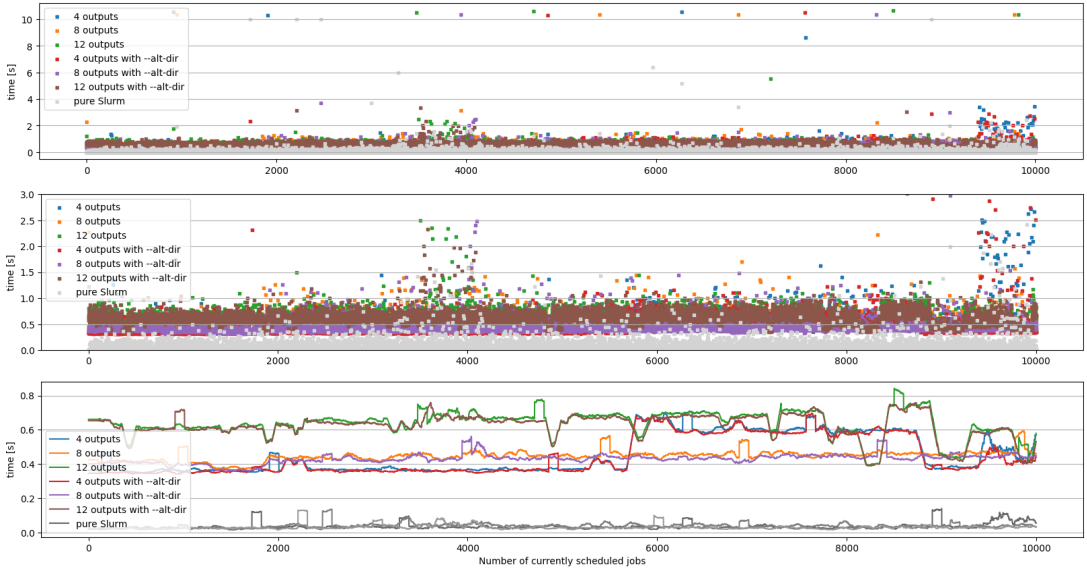
- Some overhead of 0.5*s* … 1.5*s* per job over pure Slurm
- … cost of data version management and machine-actionable reproducibility

- Adverse interaction of git with parallel file system (here GPFS)
- Increasingly slow for large repositories with $\geq$ 50 000 files
- Does not happen on local file systems

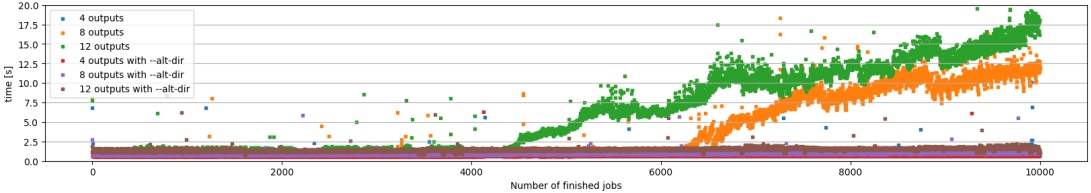
Introduce the `--alt-dir` option

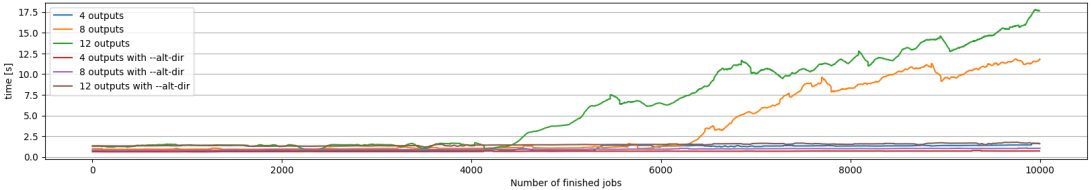
- Data repository on a local file system on a login node
- DataLad copies all input files to parallel file system as part of `slurm-schedule`
- … and copy all output files back during `slurm-finish`

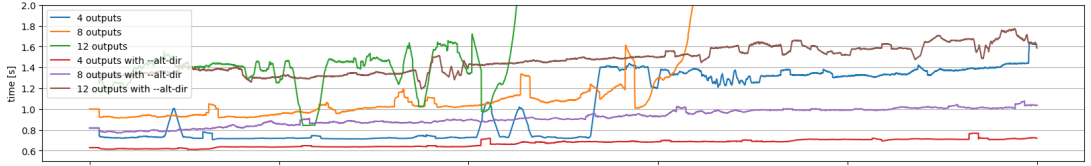
Evaluation: datalad slurm-schedule –alt-dir



Evaluation: datalad slurm-finish –alt-dir







Evaluation: datalad slurm-finish with –alt-dir

- Resonable overhead with `--alt-dir`
- basically the cost of new functionality

- Future work: Extensive evaluation on Lustre and Weka
- Future work: Evaluate with different file sizes

Summary & Outlook

Summary
- Data version control solution DataLad
- 100% git look&feel, keep existing know-how and command line / GUI / IDE tools
- Now compatible with HPC

More
- DataLad Slurm extension forbids conflicting jobs (details see paper)

Future work
- Compare with `git worktree` on parallel file systems, find out which is favorable for different scenarios
- Evaluate S3 as DataLad annex storage in HPC environments

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