

a)



```
# perform and capture a computational execution
$ datalad containers-run \
  -m "Compute subject ${subid}" \
  -n cat \
  --input "inputs/${subid}/*T1w.nii.gz" \
  --output "${subid}" \
  "<arguments for container invocation>"
```

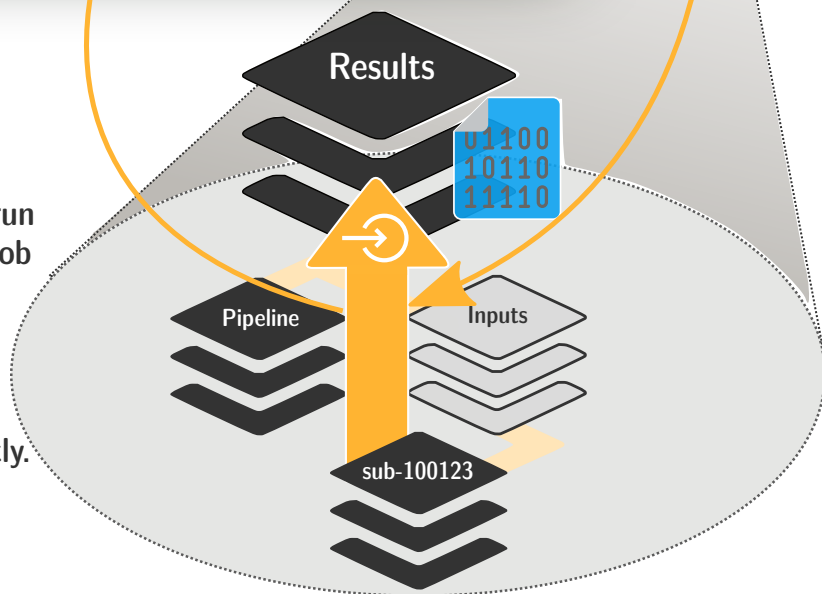
b)



```
# recompute a previous computation
$ datalad rerun e035f896s45c9
```

c)

A datalad containers-run call in each compute job performs file retrieval, computation, and provenance capture. A datalad rerun call can reproduce it exactly.



d)

commit e035f896s45c9fac70cn7cc4dbd0dad43907755p

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AuthorDate: Wed Feb 10 18:05:30 2021 +0100

Commit: Jane Doe <j.doe@fz-juelich.de>

CommitDate: Wed Feb 10 18:05:30 2021 +0100

[DATALAD RUNCMD] Compute sub-6025043/ses-2

=== Do not change lines below ===

```
{
  "chain": [],
  "cmd": "singularity exec -B {pwd} --cleanenv code/pipeline/.datalad/
        environments/cat/image sh -e -u -x -c [...]"
  "dsid": "8938de76-0302-45b5-9825-3c6ce3f3fffe",
  "exit": 0,
  "extra_inputs": [
    "code/pipeline/.datalad/environments/cat/image"
  ],
  "inputs": [
    "inputs/ukb/sub-6025043/ses-2/anat/sub-6025043_ses-2_T1w.nii.gz",
    "code/cat_standalone_batch.txt",
    "code/finalize_job_outputs.sh"
  ],
  "outputs": [
    "sub-6025043/ses-2"
  ],
  "pwd": "."
}
```

^^^ Do not change lines above ^^^

```
---
sub-6025043/ses-2/inforoi.tar.gz | 1 +
sub-6025043/ses-2/native.tar.gz | 1 +
sub-6025043/ses-2/surface.tar.gz | 1 +
sub-6025043/ses-2/vbm.tar.gz    | 1 +
4 files changed, 4 insertions(+)
```



Basic commit metadata

Author, Agent, Date, Time,
and Commit Message

Transformations

Command call/
Container parametrization

Software container image

Origin: <http://containers.ds.inm7.de/>
Version: dfa6d975ea8888ed33bf714c67

Input data

Origin: <http://ukb.ds.inm7.de/.../bids>
Version: 0c7f0b45140dde1d7291b1572

Expected output data/folder

Captured output data

Path, Content hash