

Solutions for Reproducible Research: Data Analytics

Sergio Maffioletti

S3IT: Service and Support for Science IT
Zentrale Informatik
University of Zurich

What is Open Science ?

“Open science is about the way researchers work, collaborate, interact, share resources and disseminate results.”

[Amsterdam Call for Action on Open Science](#)



Open Science: principles

Open Access

Open Data

Open Workflows

Results

Content

Processes



Reproducible research: Data Analytics

Develop container-based data analytics,

Provide validation procedure and data

Deploy and validate on the supporting infrastructures.



Reproducible research: Data Analytics

Develop container-based data analytics,

Provide validation procedure and data

Deploy and validate on the supporting infrastructures.



Reproducible research: Data Analytics

Develop container-based data analytics,

Provide validation procedure and data

Deploy and validate on the supporting infrastructures.



Reproducible research: Data Analytics

Develop container-based data analytics,

Provide validation procedure and data

Deploy and validate on the supporting infrastructures.



Reproducible research: Data Analytics

Technical challenges

- Heterogeneous infrastructure and technologies

Policy/Human challenges

- New practises for develop and validate reproducibility and portability



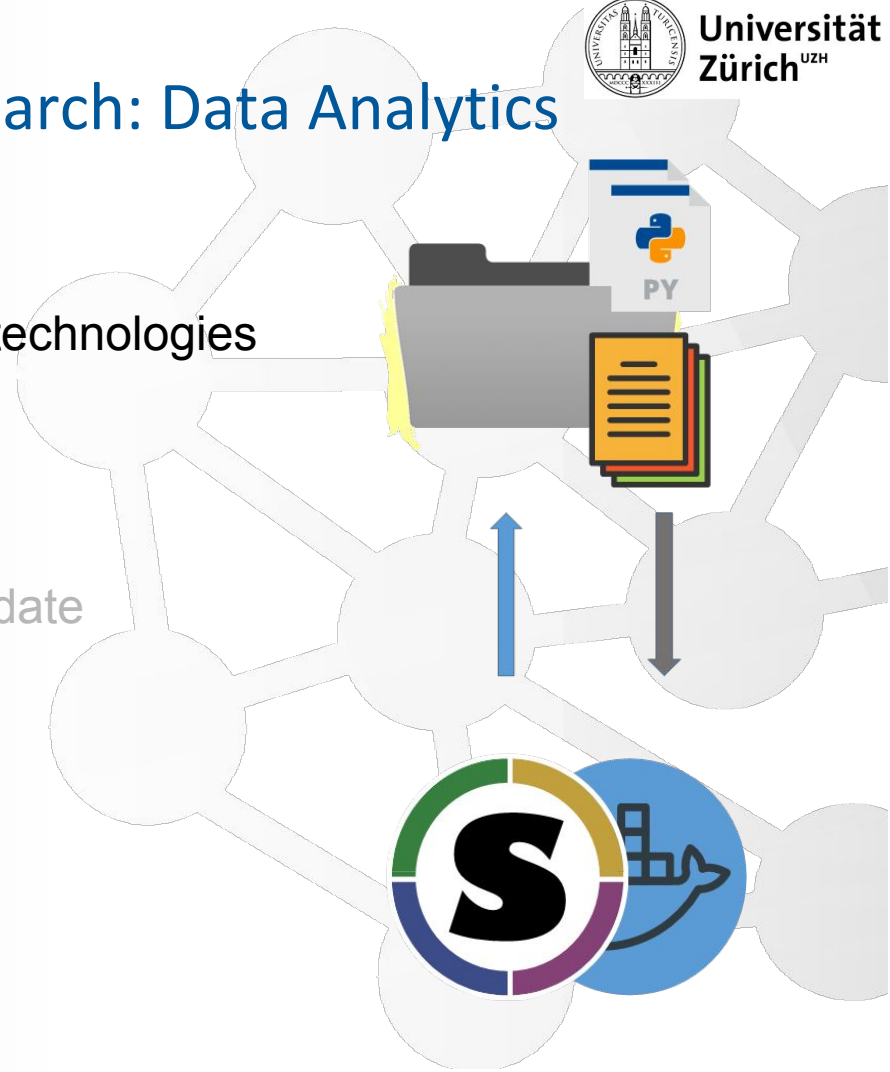
Reproducible research: Data Analytics

Technical challenges

- Heterogeneous infrastructure and technologies

Policy/Human challenges

- New practises for develop and validate reproducibility and portability



Reproducible research: Data Analytics

Technical challenges

- Heterogeneous infrastructure and technologies

Policy/Human challenges

- New practises for develop and validate reproducibility and portability



build, run and test pipelines

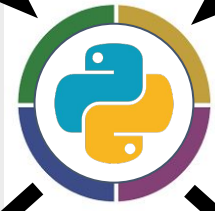
data-analysis.img



description.yaml



singularity-pipeline

**BUILD****RUN****VALIDATE**

```
name: hello_world_pipeline
version: 1
author: Balazs Laurenczy
author_org: ETHZ
substitutions:
  name: "hello_world_pipeline"
binds:
  - "/usr/lib64:/usr/lib64"
build:
  type: pull
  source: docker://blaurenczy/hello_world:latest
run:
  commands:
    - "{exec} python3 test.py > {name}.out 2> {name}.err"
test:
  validate_commands:
    - "[[ \$(md5sum {name}.out | cut -f1 -d ' ')\ \
      == \06c19b37d27dfda293492a4459fe3bc3\ ] ] && echo 0"
```

Focus on Reproducible research

- Execution environment AND data analytics workflows in containers
- Documented what's for, what goes in, what comes out
- Container's validator
 - reference dataset + expected results
- Registry of supported containers and certified providers (soon available)



Focus on Reproducible research

- Execution environment AND data analytics workflows in containers
- Documented what's for, what goes in, what comes out
- Container's validator
 - reference dataset + expected results
- Registry of supported containers and certified providers (soon available)



Focus on Reproducible research

- Execution environment AND data analytics workflows in containers
- Documented what's for, what goes in, what comes out
- Container's validator
 - reference dataset + expected results
- Registry of supported containers and certified providers (soon available)



Focus on Reproducible research

- Execution environment AND data analytics workflows in containers
- Documented what's for, what goes in, what comes out
- Container's validator
 - reference dataset + expected results
- Registry of supported containers and certified providers (soon available)



Focus on Reproducible research

- Execution environment AND data analytics workflows in containers
- Documented what's for, what goes in, what comes out
- Container's validator
 - reference dataset + expected results
- Registry of supported containers and certified providers (soon available)

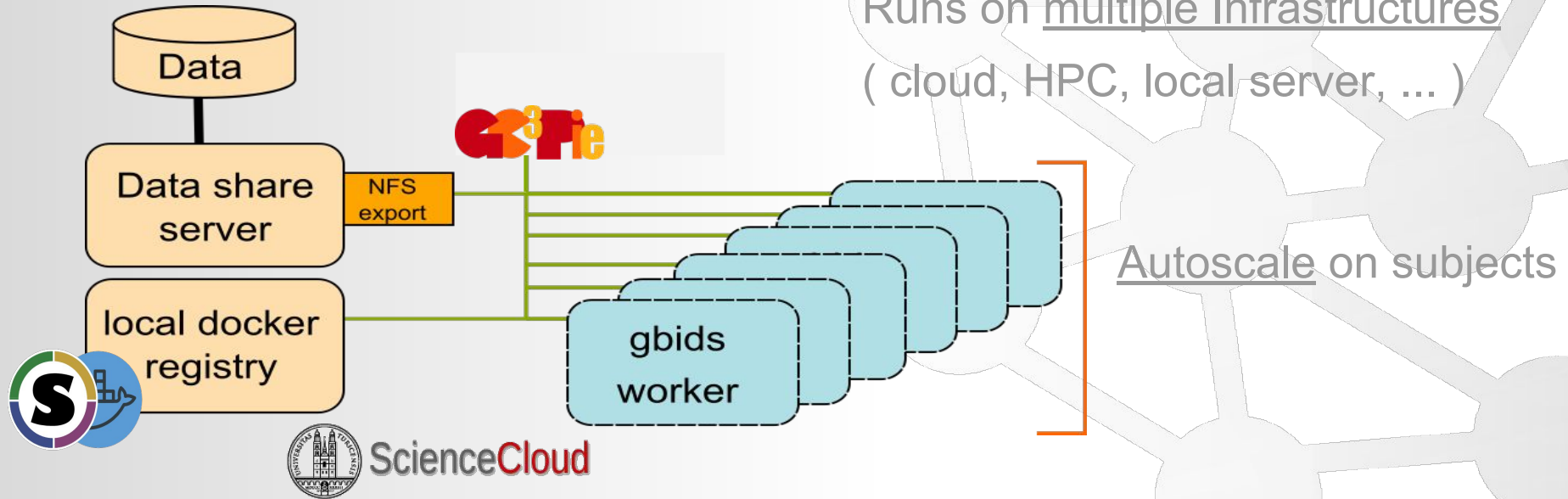


Brain imaging analysis at scale with GC3Pie

<http://gc3pie.readthedocs.io>

Support BIDS data format and apps

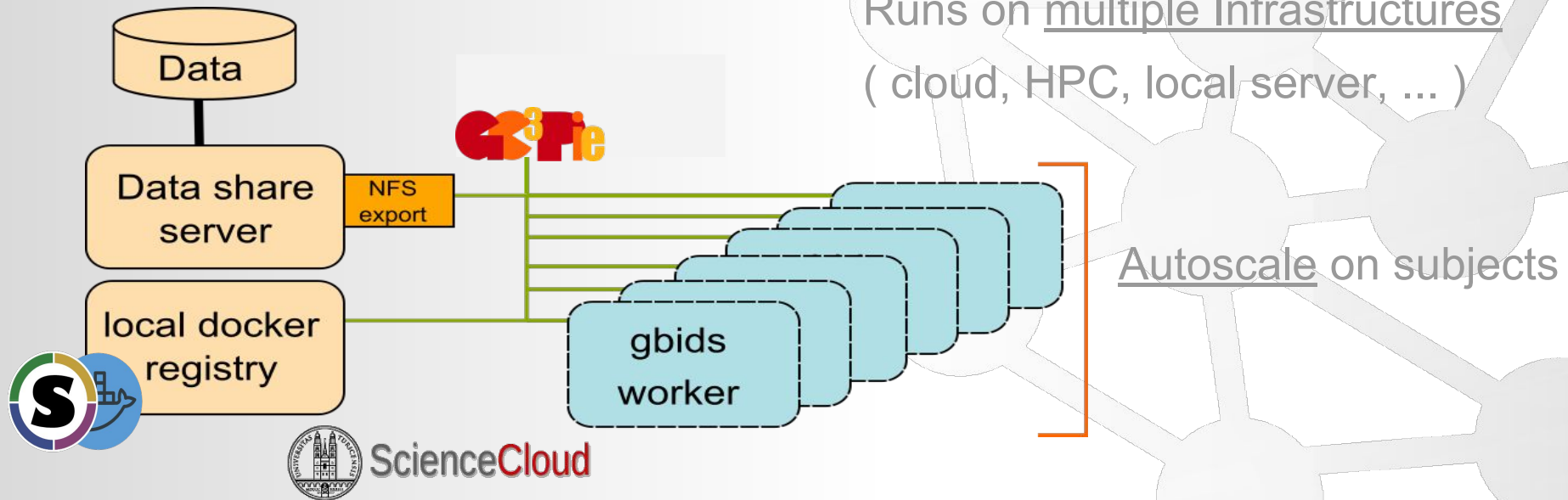
Runs on multiple Infrastructures
(cloud, HPC, local server, ...)



Brain imaging analysis at scale with GC3Pie

<http://gc3pie.readthedocs.io>

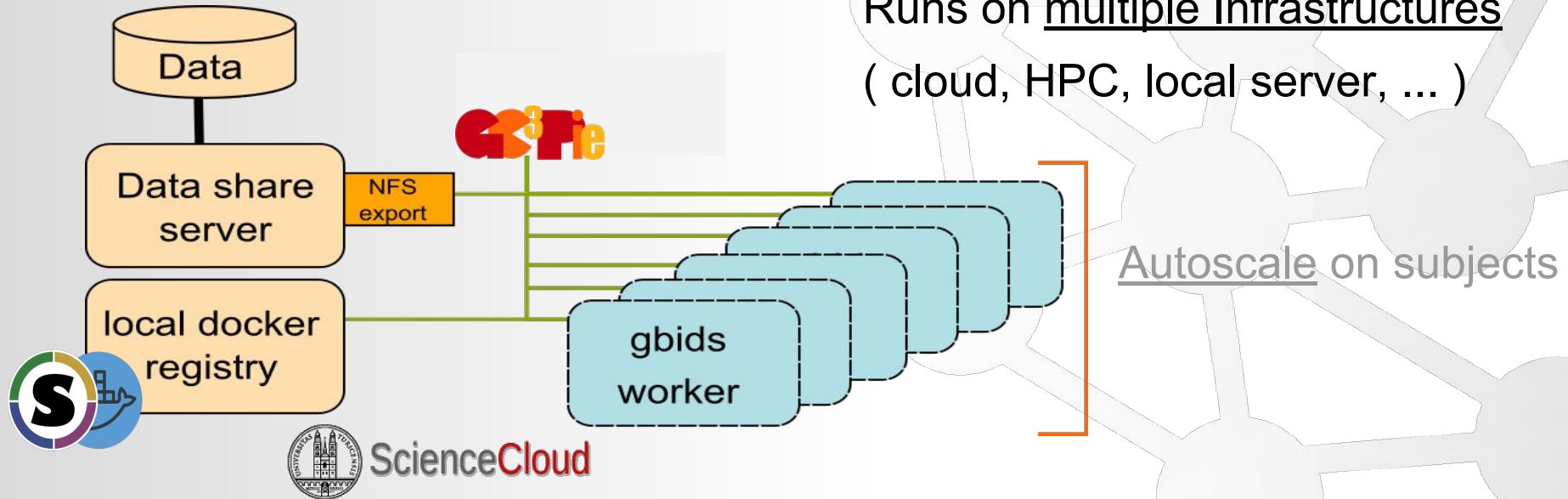
Support BIDS data format and apps



Brain imaging analysis at scale with GC3Pie

<http://gc3pie.readthedocs.io>

Support BIDS data format and apps

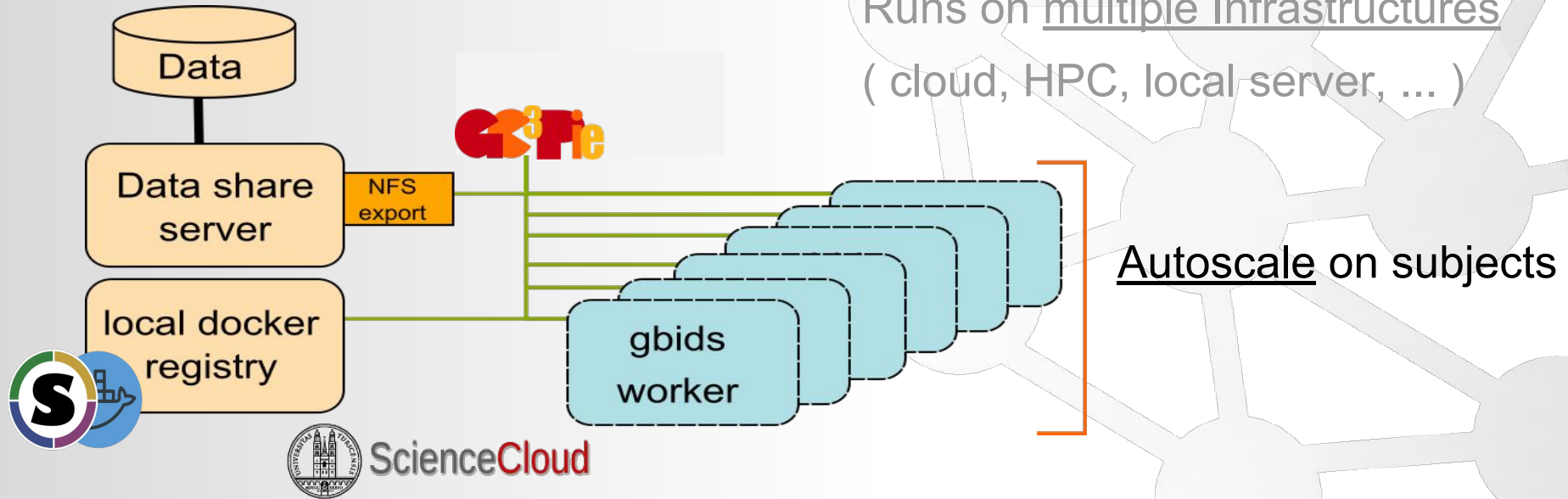


Brain imaging analysis at scale with GC3Pie

<http://gc3pie.readthedocs.io>

Support BIDS data format and apps

Runs on multiple Infrastructures
(cloud, HPC, local server, ...)



EnhanceR: enhancing Research through IT expertise

