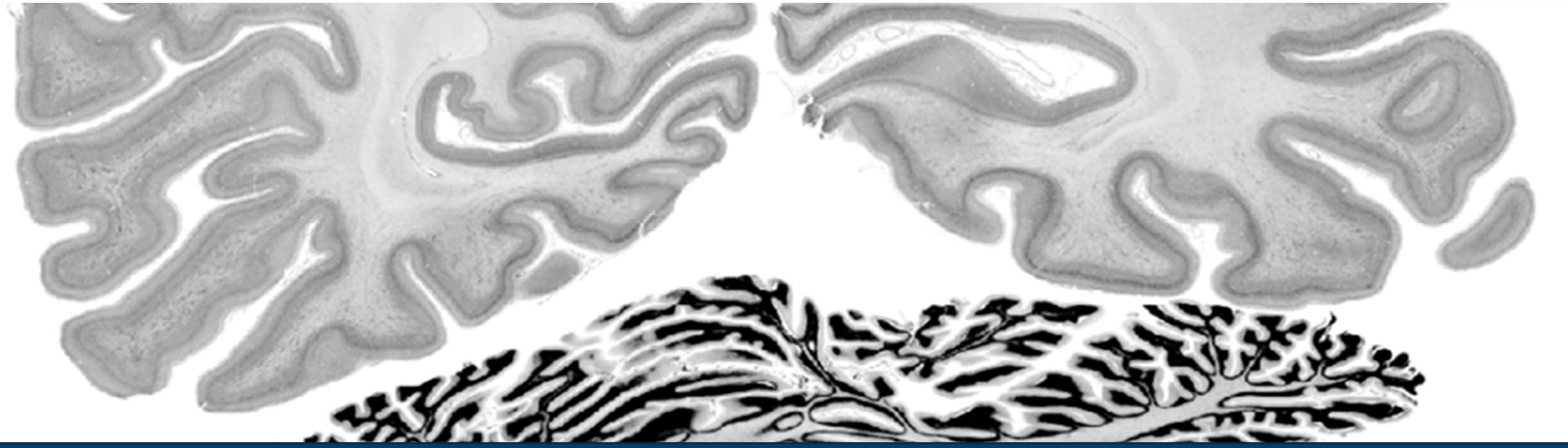

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WP4 - Connect CBRAIN & Containers to Juelich Supercomputing Centre HPC Infrastructure

Prof. Dr. – Ing. Morris Riedel et al.

3 March 2021 | Steering Board Meeting

UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES
FACULTY OF INDUSTRIAL ENGINEERING, MECHANICAL ENGINEERING AND COMPUTER SCIENCE

Mitglied der Helmholtz-Gemeinschaft

HELMHOLTZAI CIFAR Mila McGill JÜLICH Forschungszentrum

Initial Draft Architecture of Joint Infrastructure

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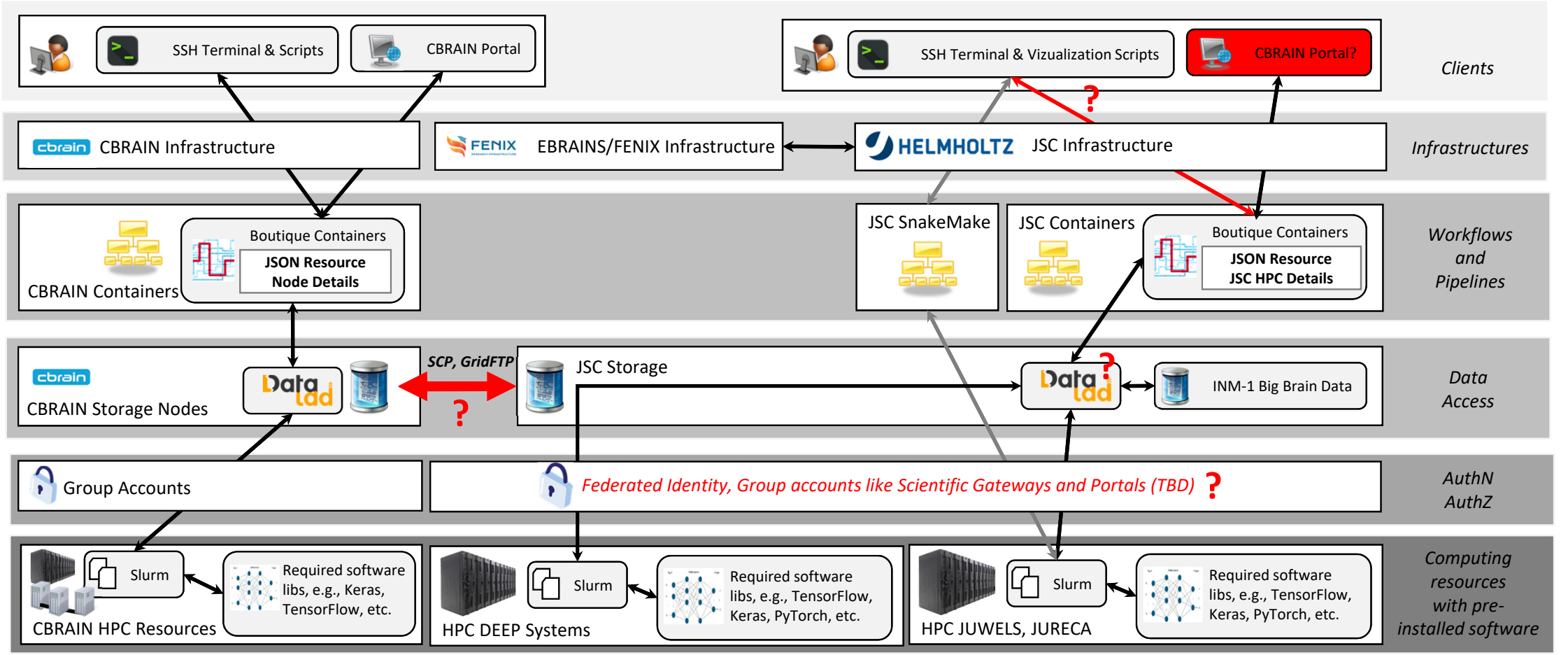

Revised Architecture of Joint Infrastructure (working)

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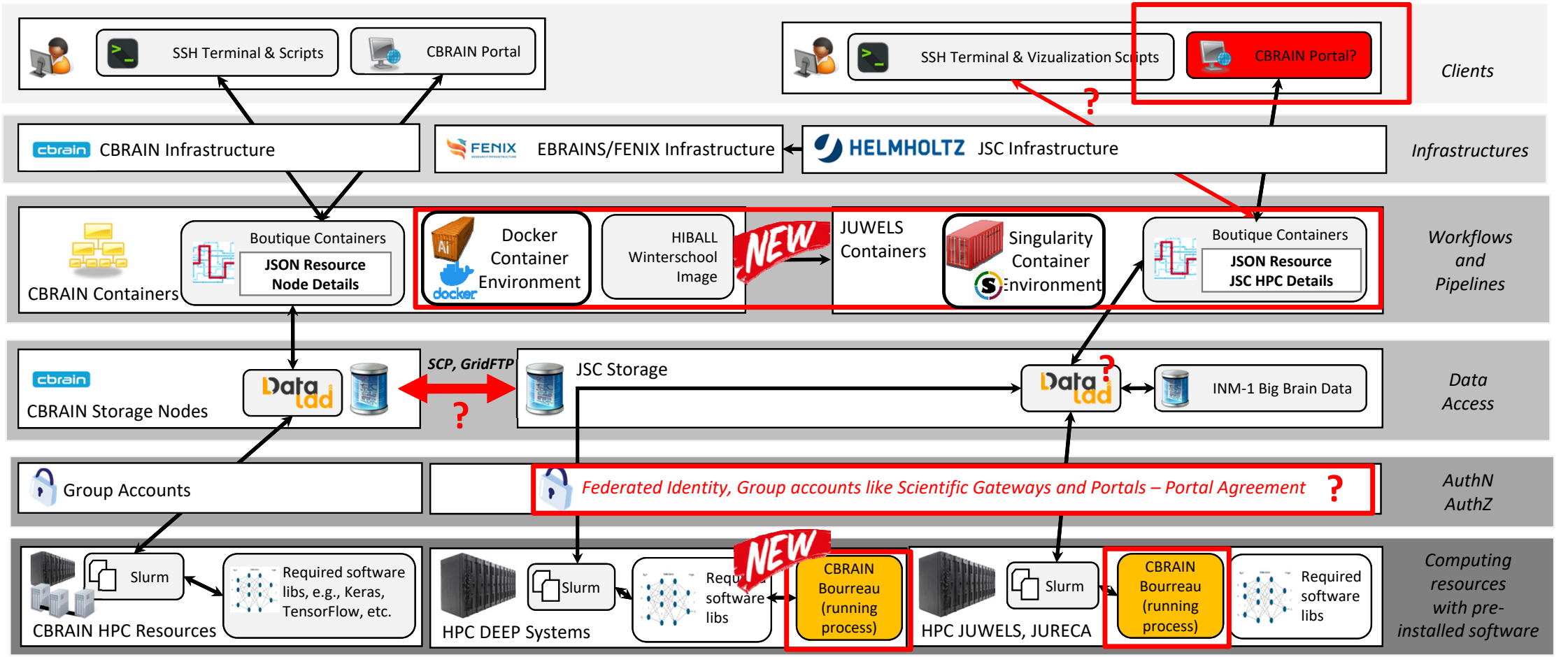

Medical AI & HPC Applications

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Covid-19 Chest X-Rays Analysis | ARDS Time Series Analysis | Neuroscience & BigBrain Research — *processing-intensive applications*

Infrastructure PRACE | EuroHPC Joint Undertaking LUMI Supercomputer | cbrain HIBALL & Canadian CBRAIN infrastructure — *computing infrastructures*

Modular HPC System DEEP - DAM | Modular HPC System JUWELS | NEW Singularity Container Environment | Docker Container Environment | Canadian CBRAIN Resource Execution | Bourreau — *innovative computing resources*

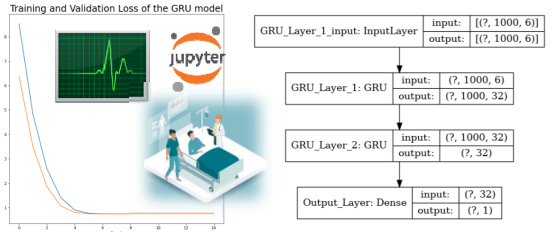
MPI & OpenMP Libraries | Distributed Training Tools (DeepSpeed) | ML/DL Libraries (TensorFlow) | JupyterLab & Jupyter Notebook Libraries | cuDNN | Git-based Data Management (Datalad) — *technology libraries & packages*

Parallel File System (Lustre) Scalable Storage Service Module | Network Attached Memory Innovative Memory Hierarchies with NVMs | Multi-core Processors (high single thread performance: ~24 cores) | NVIDIA GPUs Many-core Processors ('Accelerators' with low performance, ~7000 cores) — *key hardware technologies*

HIBALL & Neuroscience NEW

```
Some preparation
$ mkdir winterschool winterschool_cache winterschool_tmp
$ chmod +w winterschool_cache
$ export SINGULARITY_CACHEDIR=$(mktemp -d -p "$(pwd)/winterschool_cache")
$ export SINGULARITY_TMPDIR=$(mktemp -d -p "$(pwd)/winterschool_tmp")

Pull the docker image:
$ cd winterschool
$ singularity pull hws.sif docker://glatard/hws

Step into the container
$ singularity shell ./hws.sif
(the prompt changes to `>Singularity`)

download a dataset:
$ git config --global user.name "Your name"
$ git config --global user.email "peturhelgi@gmail.com"

Singularity> datalad install https://github.com/CONP-PCNO/conp-dataset.git
```

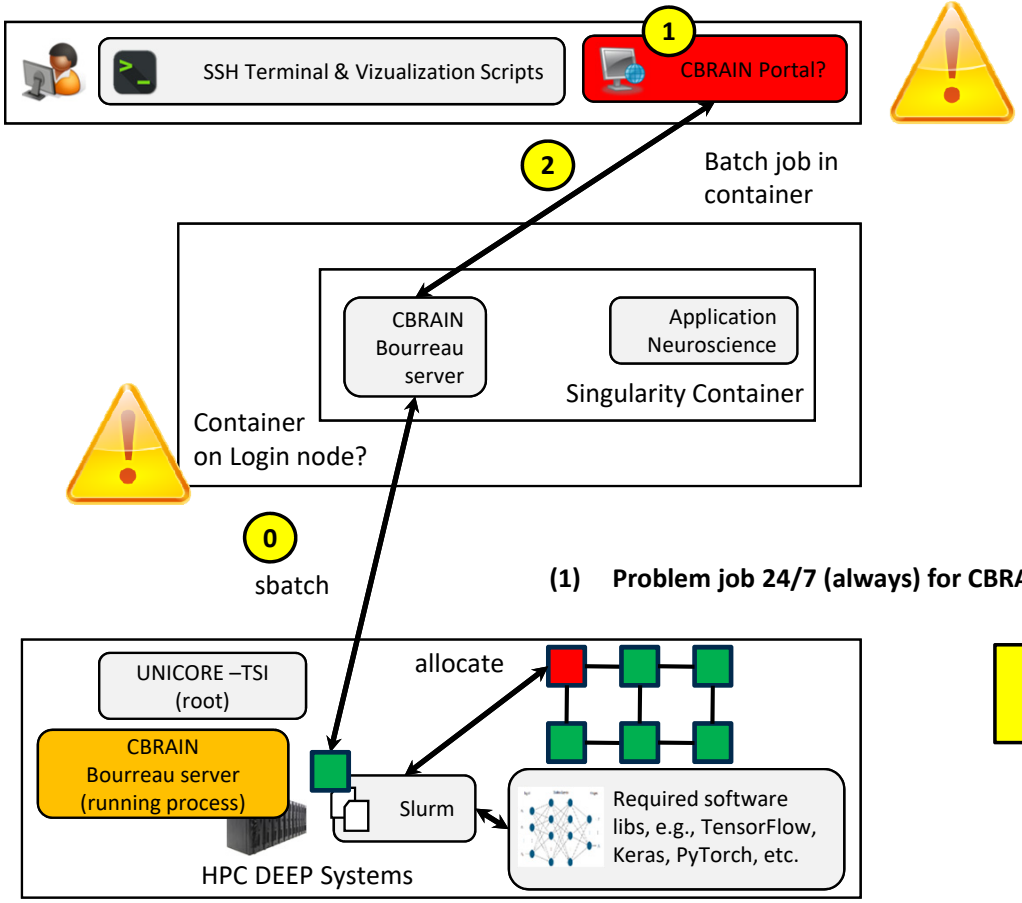
ARDS Time Series Analysis



Covid-19 Chest X-Ray Analysis


```
#!/bin/bash
# Load required modules
module purge
module use $OTHERSTAGES
module load Stages/2020
module load GCCcore/.9.3.0
module load Python/3.8.5
module load TensorFlow/2.3.1-Python-3.8.5
module load OpenCV/4.5.0-Python-3.8.5
# Activate Python virtual environment
source /p/project/training2104/ingolfsson1/jupyter/kernels/ingolfsson1_kernel/bin/activate
# Ensure python packages installed in the virtual environment are always prefered
export PYTHONPATH=/p/project/training2104/ingolfsson1/jupyter/kernels/ingolfsson1_kernel/lib
exec python -m ipykernel $@
```

Work-in-Progress – CBRAIN Executions (1)



(1) Problem job 24/7 (always) for CBRAIN Bourreau needs to listen

Not realistic!

Work-in-Progress – CBRAIN Executions (2)

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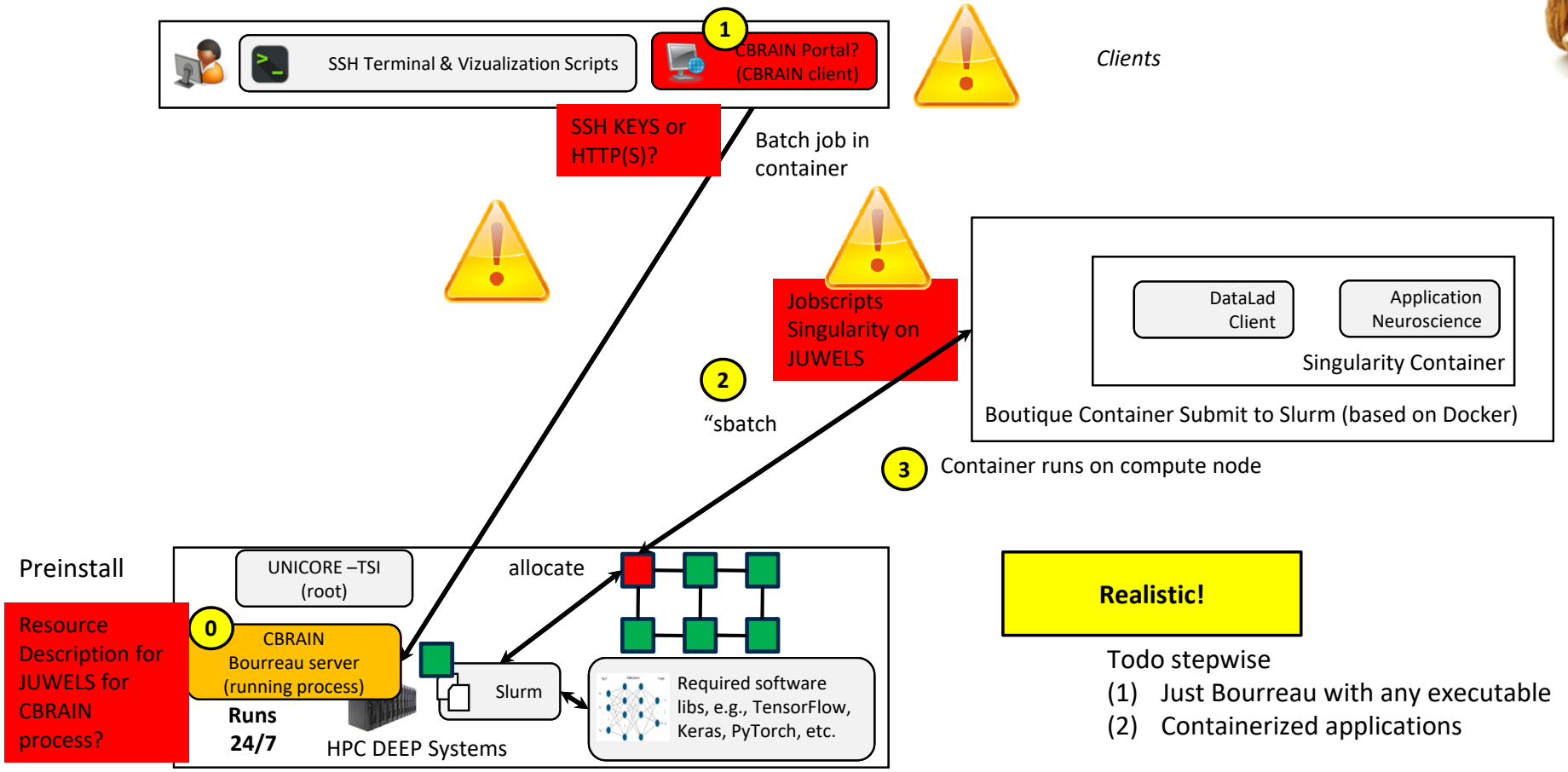

Realistic!

Todo stepwise

(1) Just Bourreau with any executable

(2) Containerized applications

Summary & Next Steps in WP4

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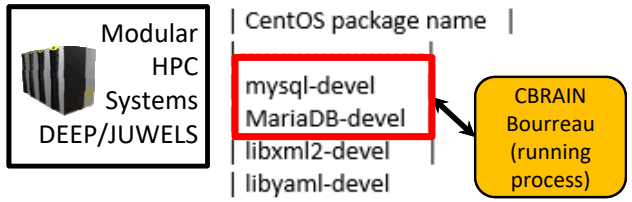
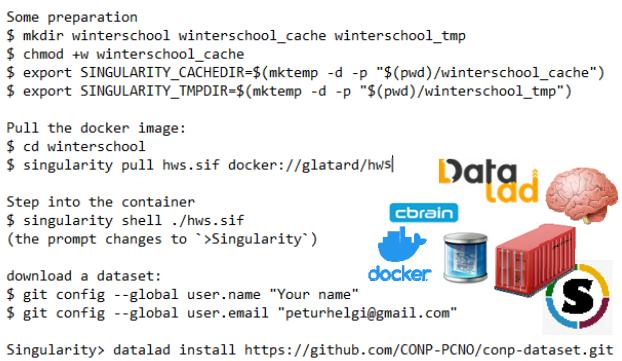
- Contributed to HIBALL Winter School
  - Preparation of Tutorial gave a big push in WP4
  - Thanks to Natacha, Tristan, Bryan, Pierre, …



- Progress in Key Fields
  - Docker containers from Tristan (Winterschool) run on JUWELS (applications within the containers work-in-progress by Petur Helgi Einarsson (UoIceland) → Tutorial Recordings



  - CBRAIN Bourreau (running process) at JUWELS/DEEP: Concept is ready, pending administrator dependencies installations, work-in-progress by Shahbaz Memon (FZJ, new in HIBALL)

CBRAIN Portal?

- Next Steps
  - Finish the CBRAIN setup & testing with Containers & portal agreement (old, see references)
  - Testing and validating complete pipelines with DataLad, CBRAIN, and Boutique containers

References

- [1] SnakeMake: https://doi.org/10.1093/bioinformatics/bts480
- [2] DataLad: https://www.datalad.org/
- [3] Boutiques: https://doi.org/10.1093/gigascience/giy016
- [4] Helmholtz HIBALL Project: https://bigbrainproject.org/hiball.html
- [5] CBRAIN: https://mcin.ca/technology/cbrain/
- [6] Portal Agreement: https://www.fz-juelich.de/SharedDocs/Downloads/IAS/JSC/EN/supercomputer/PortalOperatorAgreement.pdf?__blob=publicationFile