HPC working seminar for physicists

Scientific Computing Department at HIM

Dr. Dalibor Djukanovic

Dr. Peter-Bernd Otte

bi-weekly meeting – 10.5.2022

Today's Topics

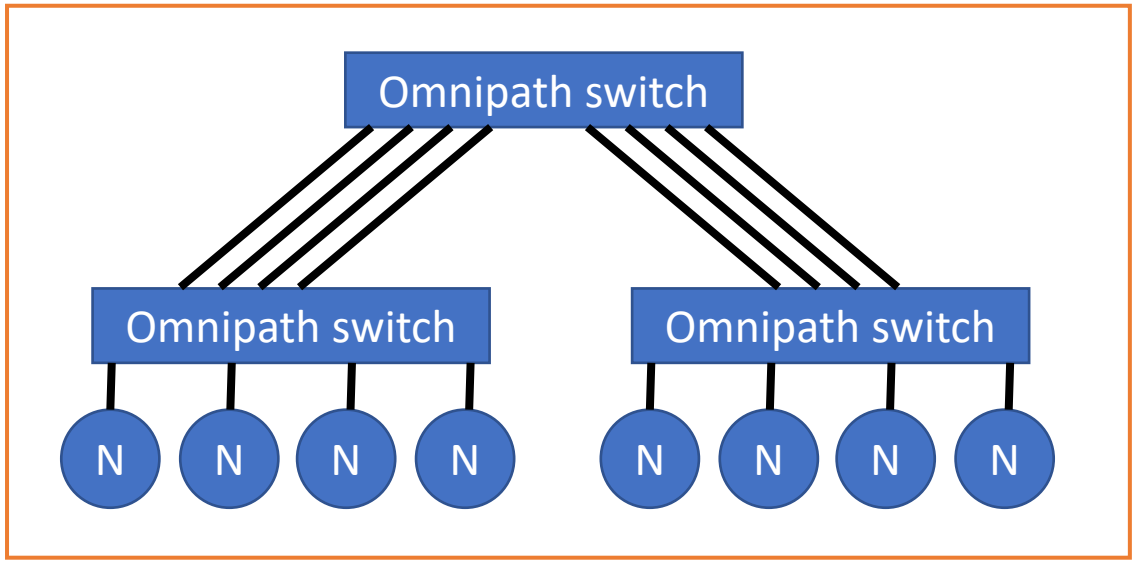
1. Himster 2: Presentations and People
2. best of tips and tricks (Himster 2 usage, singularity, CI, Jupyter)
3. your questions / discussion / requests to the maintainers

- compact in time (20mins + user questions/discussion).
- bring people together tackling the same problems
- minutes: https://www.hi-mainz.de/research/computing/hpc-working-seminar/

Presentations 2021 & 2022

- AG Denig BES III: Detector Simulation & Data Analysis
  - Christoph Florian Redmer, Riccardo Aliberti, Yasemin Schelhaas, Thomas Lenz, Max Lellmann, Yuping Guo, Tong Liu, Yaqian Wang, + MSc + BSc
- MESA: Beam Dynamics
  - Sebastian Taubert
- EMP Panda: Detector Simulation
  - Luigi Capozza, Dong Liu, Sahra Wolff, Alexander Greiner, Julian Moik
- AG Bacca Nuclear Theory Group: Precision calc. of few-body and many-body systems
  - Bijaya Acharya, Joanna Sobczyk, Limone Li Muli, Francesca Bonaiti
- SPECF-Hyp Panda: Detector Simulation & Data Analysis
  - Sebastian Bleser, Michael Bölting, Martin Christiansen, Falk Schupp, Marcell Steinen
- THFL: Nucleon form factors from lattice QCD
  - Miguel Salg

Mogon 2 ⇔ Himster 2



HPC-Gate
(PrivacyIdea)

head nodes 1..3

Mogon 2:
80% of compute nodes & interconnect

GPU
nodes

home directory

Himster 2:
320 compute nodes & Fat tree interconnect

LUSTRE

Further shared:
- maintenance
- user software
- slow control

shared

Non shared hardware

Software (1/2): Modules on Himster

14.9.2021

- echo $MODULEPATH
- export MODULEPATH=$MODULEPATH:/cluster/him/modulefiles/
- module avail
  - Remarks: D = standard module, aliases exist, L = loaded

- module avail 2>&1 | wc -l
- module load tools/Singularity/
- module list

Jupyter on headnode with plain python

28.9.2021

usage:

1. ssh himster2
2. [pbotte@login23 ~]$ source testjupyter/bin/activate
3. (testjupyter) [pbotte@login23 ~]$ jupyter notebook
4. Open locally: http://localhost:12345
   - Enter the code presented in terminal

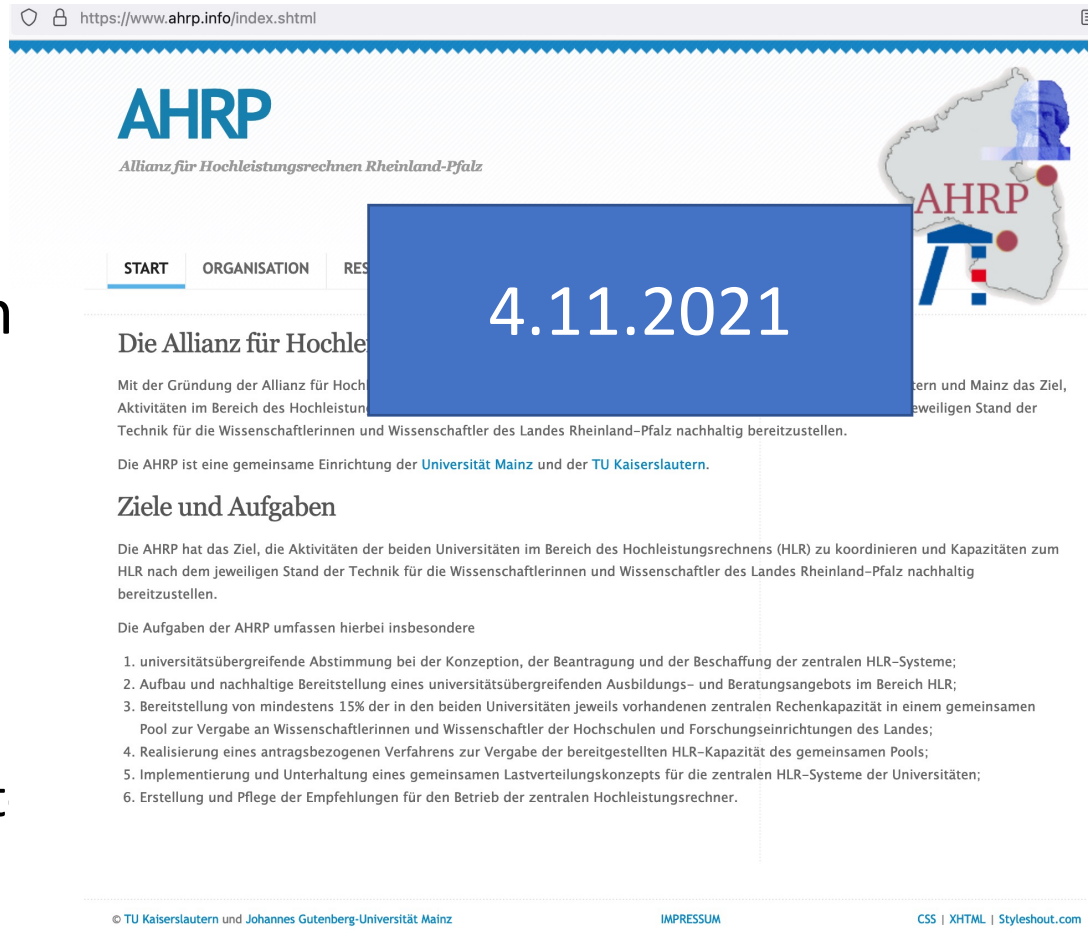
- Caution:
  - others might already use port 8888.
  - If port already in use, change config file and the port forward in SSH.

JupyterHub @ ZDV

- https://jupyterhub.zdv.uni-mainz.de
- 5*4 CPUs with 5*12GB RAM
- Intended for teaching
- For research: Solution with Mogon 2 will follow

Apply for GPU nodes

- GPU nodes only available on Mogon2, belon to University
- https://www.ahrp.info/
  - → Ressourcen
  - Antrag auf Nutzung eines rheinland-pfälzischen Hochleistungsrechners
  - (ENGLISH VERSION: Application for Using a Rhineland-Palatinate High Performance Comput
- Fill out application,
  together with 1-2 sides of project description
- Technical contact person: fill in my name (but contact me first)



Archiving Service on Himster 2/Mogon 2 (1/2)

DMP (data management plans) necessary for founding program

- Experts: https://researchdata.uni-mainz.de

9.11.2021

IRODS

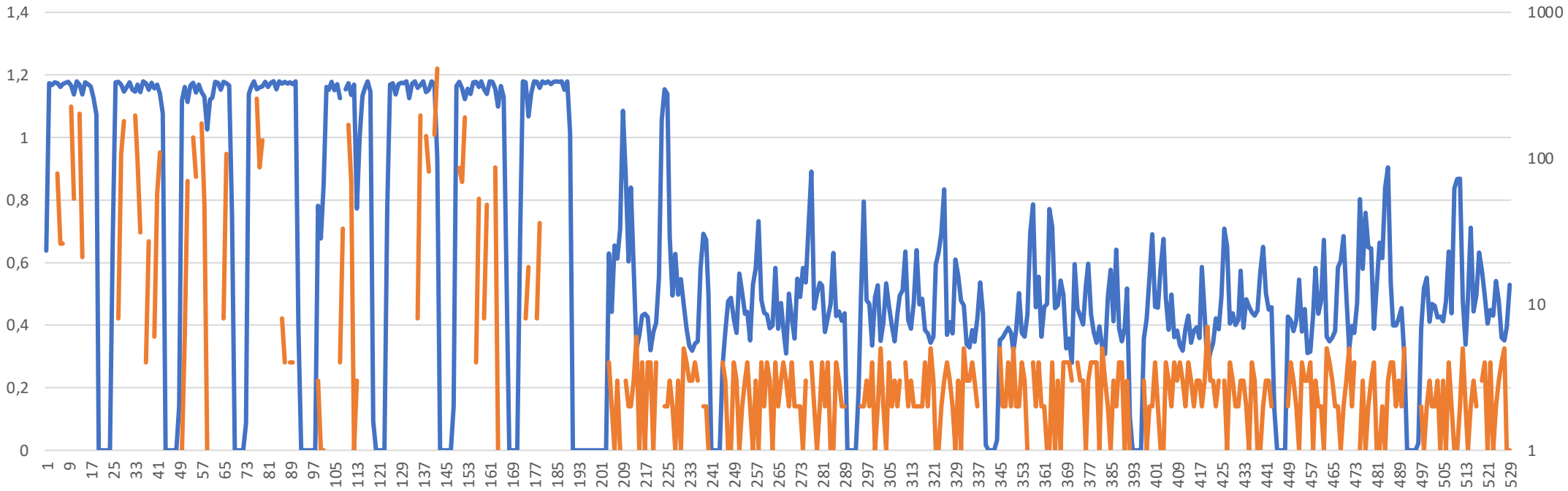
- Archiving service connected to Himster 2
- No space limit (if >1TB inform support first)
- <250TB/user -> free
- combine files until they are lager than 10GB

- Idea:
  - write once, read from time to time
  - share your raw data together with paper (measurement or analysis VMs)

Tbit Link HIM <-> GSI

GSI Test Lustre File System mounted in Mainz, same da
locally. IOR: 1.0GBytes/s write, 1.1 Gbytes/s read

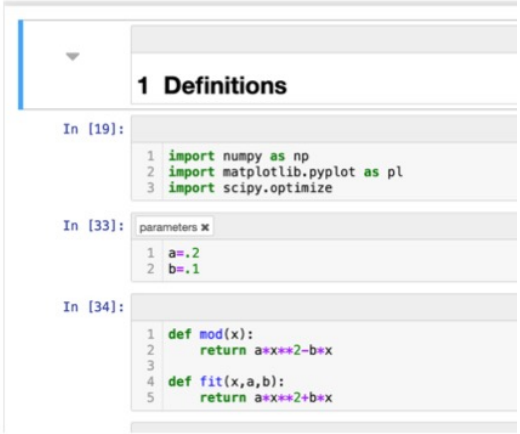
23.11.2021



Papermill

- Idea of papermill
  - Have a „template“ notebook
  - Declare parameters as input
  - Run the template notebook with input parameters
  - Save the output in a new notebook
- Example:
  - Template notebook template.ipynb
  - Two paramaters: a and b
  - Run in command line

25.1.2022




```
(venv) [djukanov@login21 papermill]$ papermill template.ipynb run1.ipynb -p a 2.2 -p b 2.55
Input Notebook:  template.ipynb
Output Notebook: run1.ipynb
```

Containerised Analysis

- Easiest way to freeze your analysis and run it again at any later time
- Same analysis on all machines
  (HPCs, around the world, workstation)
- easy start for new students

- Singularity (no Docker @ HPC)
- Try it first on your office computer
  - https://sylabs.io/guides/3.0/user-guide/quick_start.html
- Recent example:
  - BDSIM for MAMI: https://gitlab.rlp.net/-/snippets/3010

Worked out example: BDSIM with Singularity

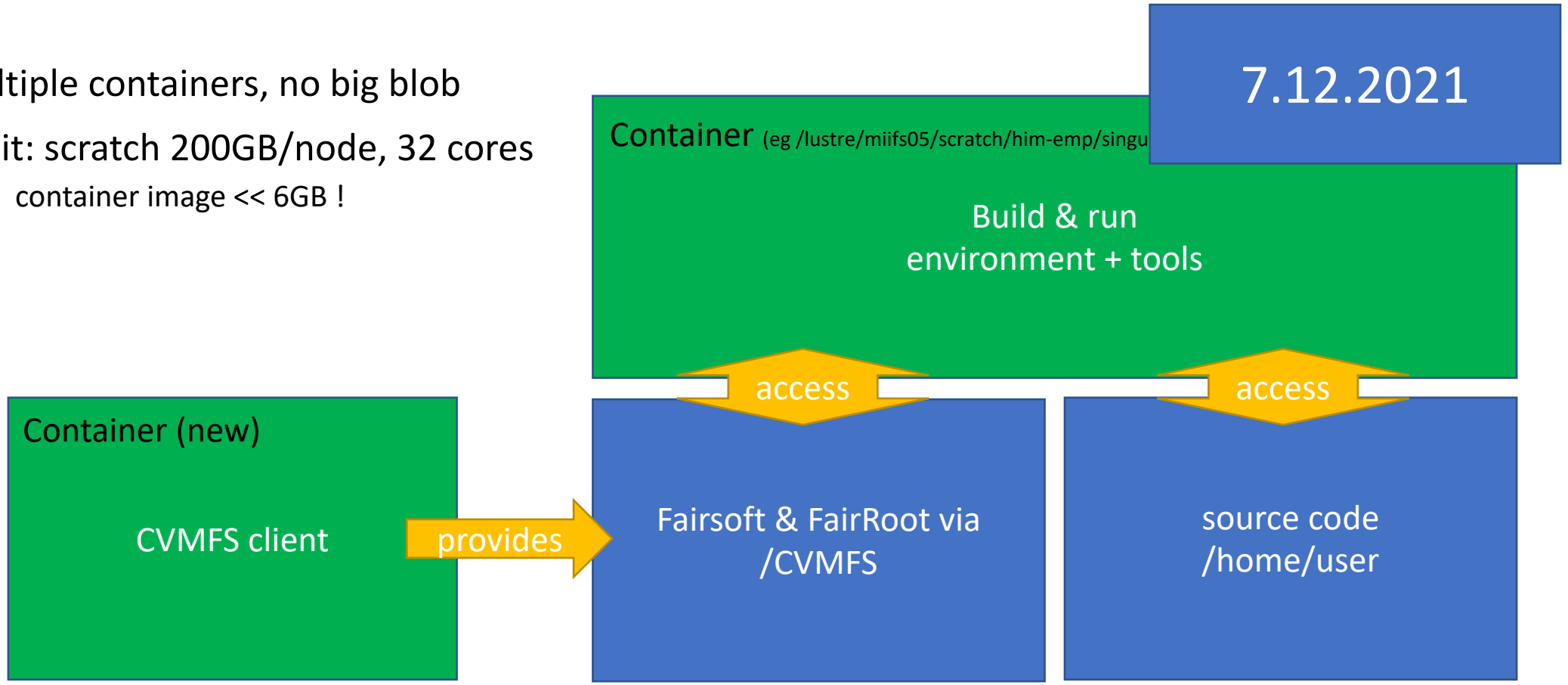
- physical setup is described in files on your home directory.
- Analysis framework (Root, Geant, …, BDSIM) sits in singularity-image: /lustre/miifs05/scratch/him-acid/singularity/bdsim.sif

- Call:

```
#!/bin/bash
#SBATCH -A m2_him_exp                # Specify allocation to charge against
#SBATCH --partition=himster2_exp.    # Queue name 'smp' or 'parallel' on Mogon II
#SBATCH --time=24:00:00.             # Run time (hh:mm:ss)

#Load the Singularity module
module load tools/Singularity

#if image is >250MB, change the TMP dir to prevent a overfull /tmp directory on node
SINGULARITY_TMPDIR=/localscratch/${SLURM_JOB_ID}/singularity_tmp/
export SINGULARITY_TMPDIR
mkdir -p $SINGULARITY_TMPDIR

singularity exec /lustre/miifs05/scratch/him-acid/singularity/bdsim.sif /bin/bash -c \
'source /local-tmp/bdsim-build/bin/bdsim.sh && source /usr/local/bin/geant4.sh && \
cd ~/bdsim-test/ && \
bdsim --file=positronBeamline.gmad --batch --ngenerate=1000 --outfile=output'
```

Containerised Analysis

- multiple containers, no big blob
- Limit: scratch 200GB/node, 32 cores
  - container image << 6GB !



Presentation by Roman Klasen on 7th December for PandaRoot analysis

CI with gitlab.rlp.net

15.3.2022

- GitLab:
  - extensive web service for source code management
  - git, wiki, issue tracking, continuous integration & deployment
- details: https://www.zdv.uni-mainz.de/gitlab/

- Limits:
  - maximal 100 projects/user
  - max. 10 GB /project
  - gitlab runner:
    - 3 VMs, each 2vCPU and 4GB RAM
    - 1h timeout
  - Shared with all on campus

- Status: 27.1.2022

Simple test

- Tests automatically run, when file “.gitlab-ci.yml” exists.

Fails:

```
image: alpine:latest

test_simple:
script:
- exit 1
```

works:

```
image: alpine:latest

test_simple:
script:
- exit 0
```

Python test (1/2)

- Use gitlab example
- Your repository gets automatically included

```
image: python:latest

# Change pip's cache directory to be inside the project directory since we can
# only cache local items.
variables:
PIP_CACHE_DIR: "$CI_PROJECT_DIR/.cache/pip"

# If you want to also cache the installed packages, you have to install
# them in a virtualenv and cache it as well.
cache:
paths:
- .cache/pip
- venv/

before_script:
- python --version # For debugging
- pip install virtualenv
- virtualenv venv
- source venv/bin/activate

test:
script:
- python hello.py
```

Python test (2/2)

- Dependent on return value of hello.py

CI fails:

```
import sys

print("Hello")

sys.exit(1)
```

CI works:

```
import sys

print("Hello")

sys.exit(0)
```

Advanced example: CI for BES3

Ingredients:

1. Docker image (CERN CentOS 7 + build environment + BES3-CVMFS)
   https://gitlab.rlp.net/bes3-mainz/CI/bossdocker/
2. CI definition file builds the docker image (standard)

3. CI definition file in analysis repository (build generator +)
   https://gitlab.rlp.net/bes3-mainz/generator/phokhara/-/blob/CI_integration/.gitlab-ci.yml

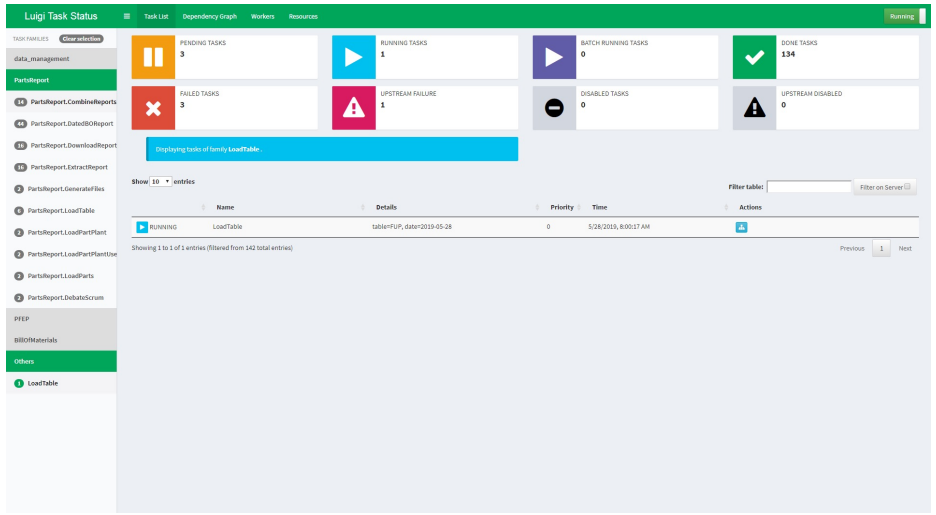
Work by Riccardo Aliberti & Thomas Lenz

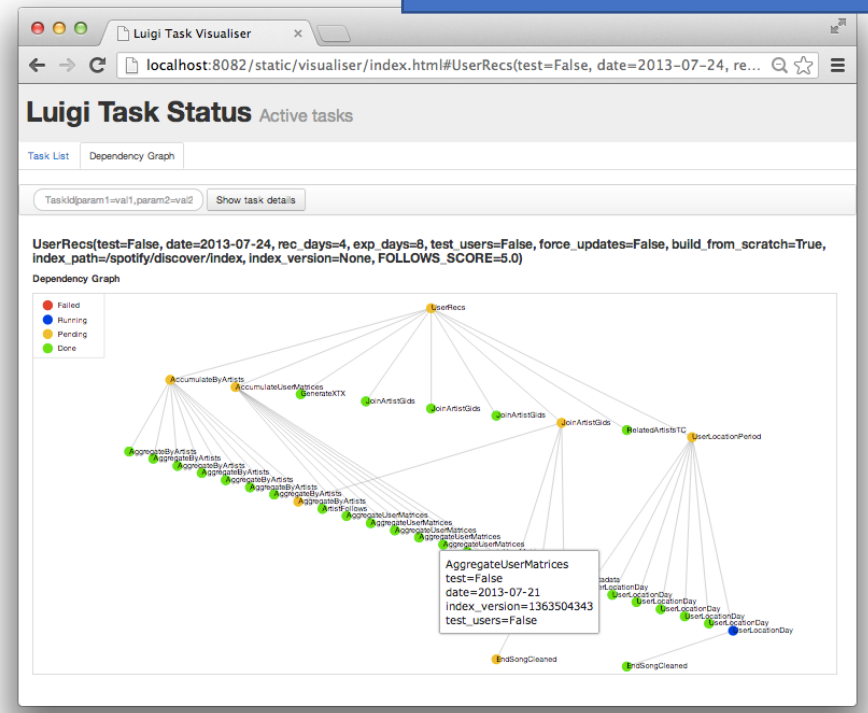
Alternative Workflow manager

https://github.com/spotify/luigi

29.3.2022

pip install luigi



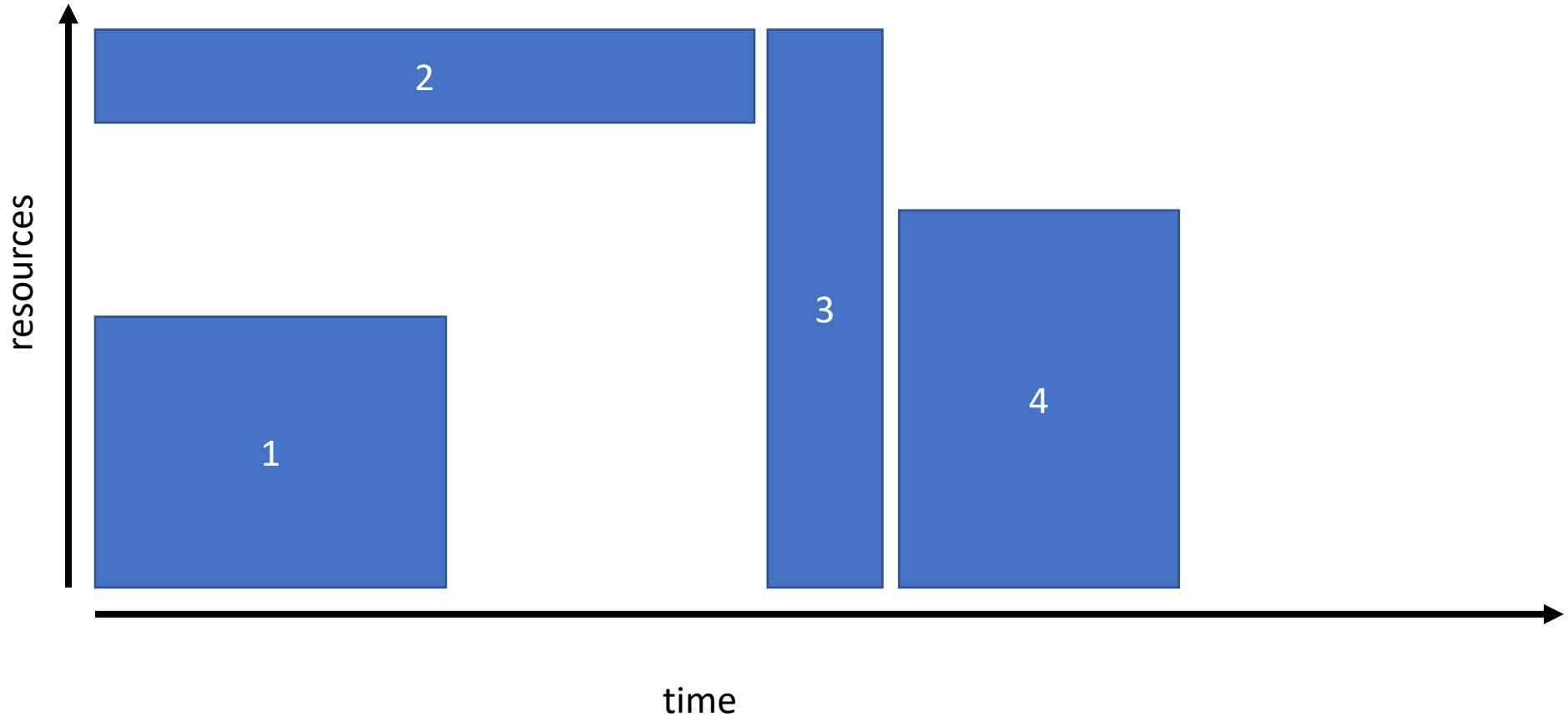


Dependency graph manger

SLURM scheduler: Multifactor Priority

26.4.2022

https://slurm.schedmd.com/priority_multifactor.html

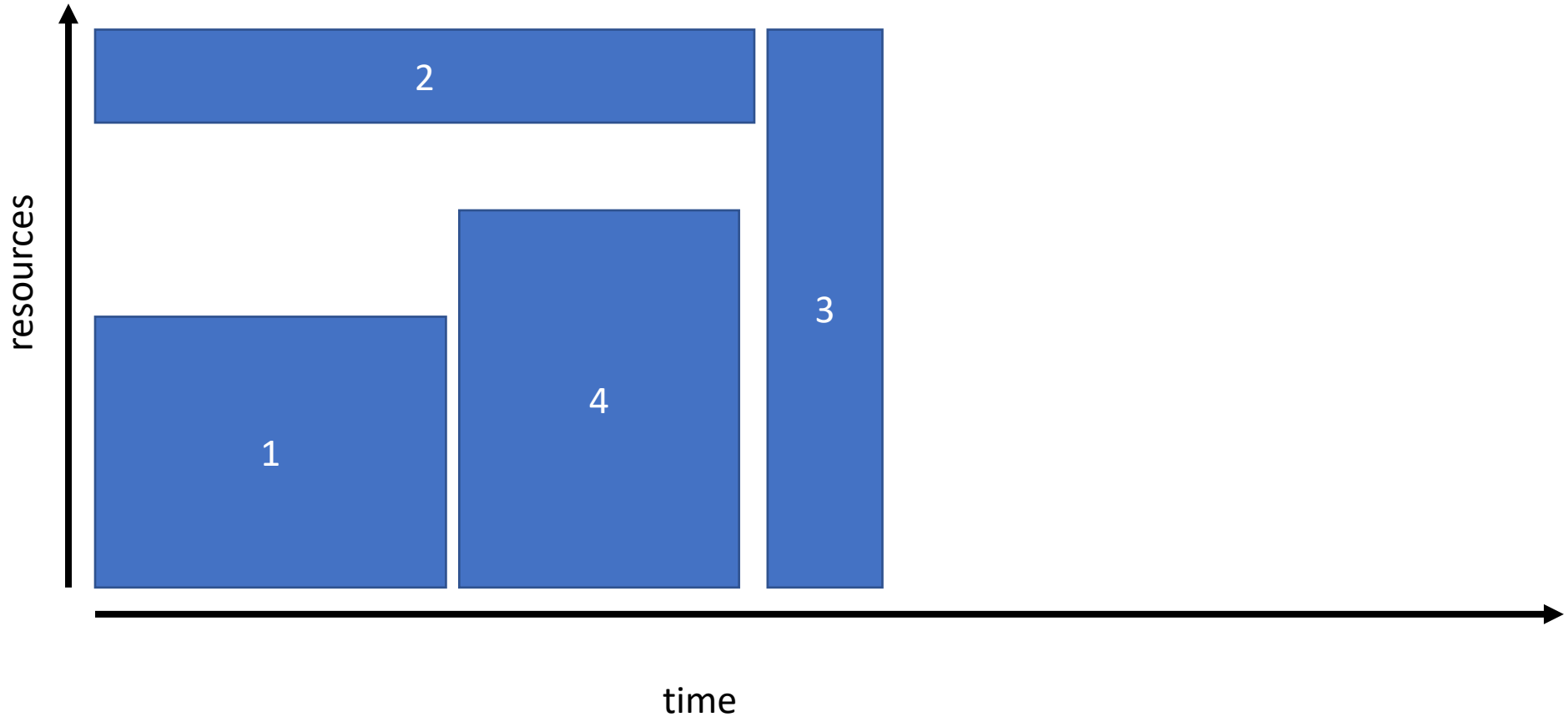


26.4.2022

SLURM scheduler: Backfilling

Performed only when jobs with higher prio are not affected

https://slurm.schedmd.com/sched_config.html



Hints (2/2)

- Use devel queue from Mogon2
- Reserve only as much resources as necessary
- Reserve resources with salloc, use them later several times with srun

- Ask for a (recurring) reservation
- Alter SLURM parameters?
- Developer node on Himster 2 exp?

your questions / discussion / requests to the maintainers?

Next meeting, 24th May 2022

- hand in your topics!

- Check out www.hi-mainz.de/tfp22