

# HPC working seminar for physicists

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# Today's Topics

1. nodes availability
2. singularity for your analysis? pros and cons

Questions to the users:

3. vote for best time slot: <https://terminplaner4.dfn.de/Ini4dhZWEVrOHwiH>
  4. your questions / discussion / requests to the maintainers
- compact in time (15mins + user questions/discussion).
  - bring people together tackling the same problems
  - minutes: <https://www.hi-mainz.de/research/computing/hpc-working-seminar/>

# Nodes availability

- large number of nodes currently in drain state:

```
[pbotte@login23 ~]$ sinfo -p himster2_exp
```

```
PARTITION    AVAIL  TIMELIMIT  NODES  STATE NODELIST
himster2_exp  up 5-00:00:00    14 drain* x[0755-0756,0759-0768,2003,2019]
himster2_exp  up 5-00:00:00    30  mix x[0753-0754,0757-0758,0769,0780-0794,2001-2002,2004-2008,2014,2020-2021]
himster2_exp  up 5-00:00:00    16 alloc x[0770-0774,2009-2013,2015-2018,2022-2023]
himster2_exp  up 5-00:00:00     5  idle x[0775-0779]
```

- Fix by ZDV applied, your response?

# Singularity for your analysis

- When NOT to use Singularity:
  - Some quick analysis that is only needed for one week.
  - AND has no dependencies.
- For everything else: use Singularity
  - reproduceable results over time (even years!)
  - on any machine (across multiple computers and HPC)
- Recent example:
  - BDSIM for MAMI: <https://gitlab.rlp.net/-/snippets/3010>
- How to get started:
  - Try it first on your office computer
    - [https://sylabs.io/guides/3.0/user-guide/quick\\_start.html](https://sylabs.io/guides/3.0/user-guide/quick_start.html)
  - Ask us for assistance.

# 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 Mogan 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'
```

# Hot Topics we are working on

- Lustre mount GSI <-> HIM via T-Bit Link
  - Test IP-connection with 10GBit/s
  - user and group mapping
- Storage upgrade for theory partition

# Next meeting, 22th February 2022

- hand in your topics!
- 23.2.—24.2.2022 Mogon / Himster 2 maintenance days