

JAN STEINER, HRZ, OCT. 20, 2023

WHAT EVERYONE SHOULD KNOW ABOUT MARVIN



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1. We can help you in many ways
2. With great (compute) power comes great responsibility
3. Common pitfalls
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1. WE CAN HELP YOU IN MANY WAYS

HOW TO GET HELP

Places to look up information:

- HPC at Uni Bonn → <https://www.hpc.uni-bonn.de>
- System-specific usage information → <https://wiki.hpc.uni-bonn.de/>
- General HPC information → <https://hpc-wiki.info> (+ Google)
- Linux command line tutorial → [https://hpc-wiki.info/hpc/Introduction to Linux in HPC](https://hpc-wiki.info/hpc/Introduction%20to%20Linux%20in%20HPC)
- How does your software interact with GPUs, MPI, etc. → software documentation

MAIN COMMUNICATION CHANNELS

- Website: <https://www.hpc.uni-bonn.de>
- Mailing lists:
 - One per system → maintenance downtimes etc.
 - All users added upon registration
 - hpcforum@listen.uni-bonn.de: general announcements (e.g. training courses), discussion

OUR TRAINING COURSES

- Multiple 1-day courses
- 3-week machine learning course
- Registration via [eCampus](#)

- Held once per semester
- Additional courses possible (e.g. for your research group)
 - contact@hpc.uni-bonn.de

TRAINING COURSE TOPICS

Basic topics (1 day each)

- Introduction to Python
- Introduction to Linux (command line)
- Introduction to Working on HPC Clusters
- Version Control with Git

Advanced course (3 weeks):

Foundations of Machine Learning

- Topics:
 - Basics (linear algebra, statistics etc.)
 - Classification and other algorithms
 - Neural networks
- Hands- on programming exercises

And more courses in development...

Consulting services

- Getting more complex software/cases to run
- Advice on which system to use (including regional and national HPC systems)
- Improve performance of your code

Two teams:

- HRZ HPC Team → Expertise on day-to-day operations and cluster use
- HPC/A Lab → Expertise in various scientific domains

HOW TO GET CONSULTING SERVICES

- Schedule consulting session
 - E-mail us: contact@hpc.uni-bonn.de
- Availability depends on our workload
- What we **cannot** do: do your work for you

2. WITH GREAT (COMPUTE) POWER COMES GREAT RESPONSIBILITY

- You are sharing a **limited resource**
- With the **entire university**
- With comparatively **few technical restrictions**
- HPC systems: expensive, high power consumption

→ We rely on you to use resources responsibly

RESPONSIBLE USE

- Only reserve resources that you need (e.g. GPUs)
 - Common: inherit job script from previous PhD student – take time to understand parameters!
- Take some time to properly configure your software
 - Avoid idling, reduce inefficiencies
- Remember: we offer support and consulting

- That said: generous reserve is in order
 - 1.5 – 2 times runtime
- Jobs get killed at time limit → better to leave time
- Job prioritization algorithm: the more you use, the less priority subsequent jobs have

3. COMMON PITFALLS

Running jobs on front end

- Usually: complete newbie who does not know better
- Slows down login node for everybody
- Instead: **job script**
 - https://wiki.hpc.uni-bonn.de/getting_started
 - https://wiki.hpc.uni-bonn.de/running_jobs
 - „Introduction to Working on HPC Clusters“ course
- OK on front end: compiling, short (!) tests

Talking to wrong software/hardware

- Common with Python
 - Multiple instances (virtual envs, Conda envs)
 - Install package into wrong instance

- Login nodes have slightly different hardware
 - No GPUs → non-GPU version of software might get installed

Not accounting for job failure

- We make no guarantee that cluster works
- Programming errors might not show until later

- Check what your jobs do
- Allow time for re-runs
- Implement checkpointing

4. OUTLOOK: THE NEXT STEPS FOR MARVIN

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- Closed testing phase begins next week
 - First actual cases will be run
- Current plan: registration and use of Marvin for all users by December
 - Registration process similar to Bonna
- In any case: new developments announced via <https://www.hpc.uni-bonn.de> and hpc-forum@listen.uni-bonn.de

THANK YOU FOR YOUR ATTENTION

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<https://www.hpc.uni-bonn.de>