

JAN STEINER, HRZ, OCT. 20, 2023 WHAT EVERYONE SHOULD KNOW ABOUT MARVIN

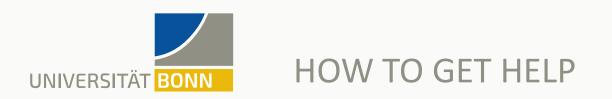




- 1. We can help you in many ways
- 2. With great (compute) power comes great responsibility
- 3. Common pitfalls
- 4. Outlook: the next steps for Marvin



1. WE CAN HELP YOU IN MANY WAYS



Places to look up information:

- HPC at Uni Bonn → <u>https://www.hpc.uni-bonn.de</u>
- System-specific usage information \rightarrow <u>https://wiki.hpc.uni-bonn.de/</u>
- General HPC information \rightarrow <u>https://hpc-wiki.info</u> (+ Google)
- Linux command line tutorial \rightarrow <u>https://hpc-</u> wiki.info/hpc/Introduction to Linux in HPC
- 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 \rightarrow maintenance downtimes etc.
 - All users added upon registration
 - <u>hpca-forum@listen.uni-bonn.de</u>: general announcements (e.g. training courses), discussion



- Multiple 1-day courses
- 3-week machine learning course
- Registration via <u>eCampus</u>
- 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

<u>Advanced course</u> (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...



IN-DEPTH CONSULTING SERVICES

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

<u>Two teams</u>:

- HRZ HPC Team \rightarrow Expertise on day-to-day operations and cluster use
- HPC/A Lab \rightarrow 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

\rightarrow We rely on you to use resources responsibly



- 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 \rightarrow better to leave time
- Job priorization 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 \rightarrow 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



OUTLOOK: THE NEXT STEPS FOR MARVIN

- 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 <u>https://www.hpc.uni-bonn.de</u>
 and <u>hpca-forum@listen.uni-bonn.de</u>



THANK YOU FOR YOUR ATTENTION

Contact:

Jan Steiner

contact@hpc.uni-bonn.de

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