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
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
- 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
  - hpca-forum@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
RESPONSIBLE USE

- 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
 RESPONSIBLE USE

− 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
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
COMMON PITFALLS

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
COMMON PITFALLS

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 https://www.hpc.uni-bonn.de and h pca-forum@listen.uni-bonn.de
THANK YOU FOR YOUR ATTENTION

Contact:
Jan Steiner
contact@hpc.uni-bonn.de
https://www.hpc.uni-bonn.de