High Performance Computing

An outlook on 2023 (and beyond) for the University of Bonn

Dr. Dirk Barbi (HRZ Uni Bonn), TeRAbytes Workshop, 18.01.2023

HPC – A central service offered by HRZ

The University of Bonn decided to implement High Performance Computing as a **central service to all scientists:**

- Extensive Hardware Resources
- In-depth Support on all Levels
- Teaching (Workshops and Courses)
- Performance Measurement and Optimization
- Counselling of HPC-related science projects
- <u>Two teams </u>to offer these services

HPC – A central service offered by HRZ

Aim:

- Accomodate for (most) needs by central installations
- Enable users to efficiently use these resources
- Support scientists with finding solutions to (technical) problems
- Possibly replace smaller, less efficient clusters, or join systems (e.g. HTC integration, extensions)

THE HPC TEAM (HRZ UNI BONN)
HPC Operations team / Basic services

Dr. Dirk Barbi

Marvin Procurement, Project
Management, Team Leader

Jan Steiner

Workshops and Courses,
User Support

Michael Kuckertz

Bender Administration,
Technician

4 Open positions
(2*E13, 2*E11)

The High Performance Computing / Analytics (HPC/A)-Lab

Prof. Dr. Petra Mutzel

Scientific director, computational analytics

Dr. Michael Hübner

Experimental high energy particle physics

Dr. Bartosz Kostrzewa

Extreme scale computing, lattice field theory

Dr. Sven Mallach

Mathematics, computer science

Dr. Malte Petersen

Bioinformatics, computational genomics

Dr. Moritz Wolter

Machine learning, artificial intelligence

Central contact point for research projects involving HPC

Interdisciplinary Collaboration

Advanced advice and training

Three pillars of services

Resources (Clusters)

- Now: Bonna, Bender

- April 2023: Marvin (huge)

- open to all scientists at the university

User Support

First-Level Support for all basic (technical questions)

Advanced and scientific questions answered by HPC/A

Teaching

Basic Workshops / Courses by HPC@HRZ

More Advanced and in-depth trainings by HPC/A

1 (Hardware) Resources

Heavy Metal

Bonna (since 2017)

Small MPP Cluster

- Maintained by Fraunhofer SCAI
- 2240 cores total (70 nodes)
- 192GB RAM / node
- Application form on hpc.uni-bonn.de

Bender (since 2022)

Small GPU Cluster for students and teaching

- 16 Nvidia A40 GPUs (in 4 nodes)
- 16 Nvidia A100 GPUs (in 2 nodes)
- Application form on hpc.uni-bonn.de

Marvin (starting 2023)

- 18432 cores in total (192 nodes), Intel Sapphire Rapids
- 1024 GB RAM / node
- 24 Large Mem nodes, 2 Very Large Mem Nodes
- 128 GPUs Nvidia A100 80 GB (32 nodes)
- 192 GPUs Nvidia A40 48 GB (24 nodes)
- 5.6 PB Lustre Filesystem

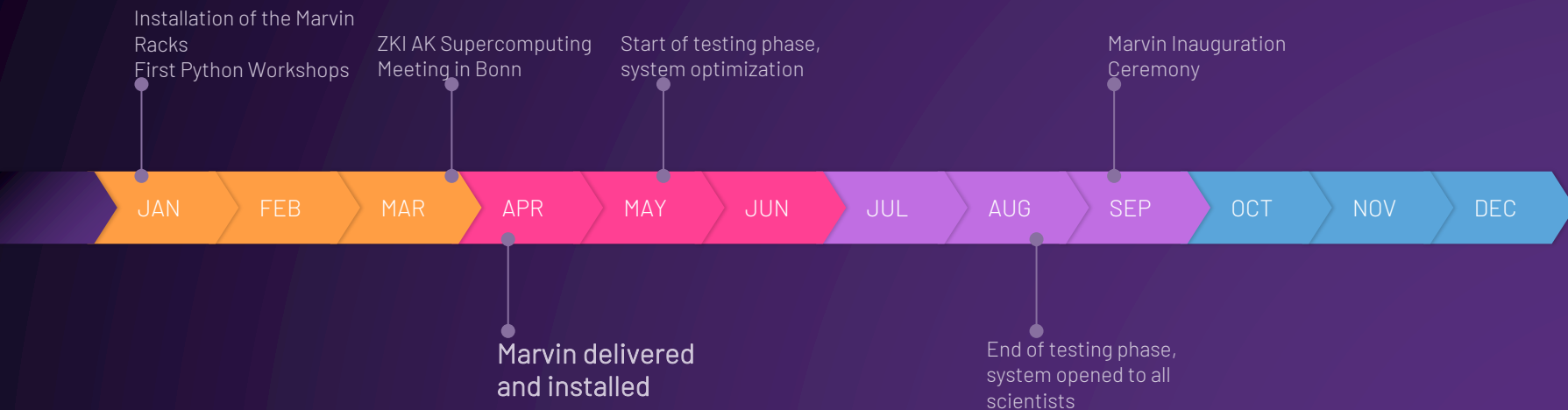To be delivered / installed in April, opened to scientists in summer 2023

Marvin's New Home

- Marvin will be installed into the INS server room
- Currently being upgraded by Abt. 4.5 to up to 600 kW max cooling / power consumption of the HPC cluster
- Racks already in place (among many other things)

TIMELINE 2023

Installation of the Marvin
Racks
First Python Workshops

ZKI AK Supercomputing
Meeting in Bonn

Start of testing phase,
system optimization

Marvin Inauguration
Ceremony

| JAN | FEB | MAR | APR | MAY | JUN | JUL | AUG | SEP | OCT | NOV | DEC |

Marvin delivered
and installed

End of testing phase,
system opened to all
scientists

2 User Support

Problem solving and Consultation

Ticket system based support, User forum

One contact point for support questions

Internally directed to the correct supporter (both teams)

Newsletter, MOTD, Regular Meetings (for Admins),...

Also: HPC Office at Wegelerstr. 6

3 Teaching

Making sure everyone knows what he/she's doing

Introductory Workshops / Courses by HRZ

Either online, as recorded tutorial, in person, or combination, i.e.:

- Python

- Linux / Shell

- VCS (git)

- Introduction to HPC

- Raspberry Pi Cluster

- C / C++

- …

Advanced Workshops / Courses by HPC/A

More in-depth topics, advanced fields, like:

- Machine Learning

- Performance Analysis and Optimization
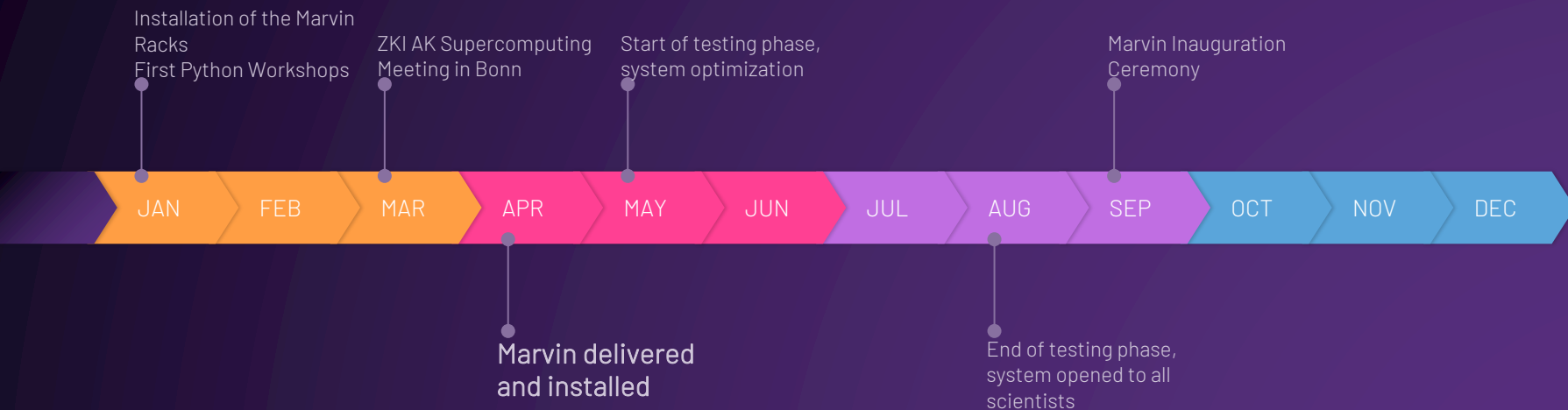
- Advanced Parallel Programming

- ...

4 Last Remarks

(If you want to remember something, then this)

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Resources

hpc.uni-bonn.de is the shared website of both HPC-teams, containing

- Information on the hardware resources, scheduled downtimes, problems etc.

- Upcoming workshops, courses, events, meetings...

- Wiki

- Useful links

- ...