News

bw|HPC

BinAC Cluster · Location: University of Tübingen

bwHPC Newsletter

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Dear bwHPC users,

we present you our bwHPC newsletter, where you will find up-to-date information on events, resources and success stories around the bwHPC-S5 project.

bwHPC team

## 7th bwHPC Symposium: bwHPC in dialogue with scientists

On November 8, 2021, Ulm University hosted the **7th bwHPC Symposium.** bwHPC stands for High Performance Computing in Baden-Württemberg. Due to the COVID-19 pandemic, the symposium was held online for the first time in its history. The declared goal of this symposium is to bring together scientists from different disciplines and the operating teams of HPC sites in Baden-Württemberg. In total, the symposium counted 147 attendees, 24 oral presentations and 13 posters.

The opening speech was given by Prof. Dr. Stefan Wesner, Chief Information Officer (CIO) of the University of Ulm. Afterwards, Prof. Dr. Wolfgang P. Schleich, the acting director of the DLR Institute for Quantum Technologies, gave a plenary lecture on quantum computing. In a more technical session, bwHPC and the associated project bwHPC-S5 (Scientific Simulation and Storage Software Services) were briefly introduced by the project management, followed by presentations on research data management and national high-performance computing from invited representatives. Subsequently, scientists provided a comprehensive program of interesting presentations from different disciplines.

Part of the symposium was also a poster session. A wide variety of topics was displayed on the posters ranging from bwHPC projects over technical concepts to concrete scientific results. The posters were placed in so called breakout rooms. During breaks in between lectures, all participants could freely roam through these rooms and discuss with each other. This concept offered an additional opportunity to get in touch with the attendees of the symposium and it was received overwhelmingly positive.

Despite the challenges caused by COVID-19, the 7th bwHPC Symposium was successful building upon its established platform of exchange between users and operators of HPC systems. The dialogue with scientists and HPC users is essential, since the benefit of new technologies can only be evaluated in close collaboration with them and the results of these discussions will eventually lead to a new productive HPC infrastructure at state level. This year, the 8th bwHPC Symposium will be held at the University of Stuttgart.
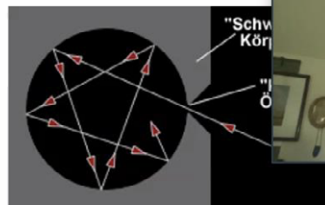
Lecture by Prof. Dr. Wolfgang P. Schleich about quantum computing
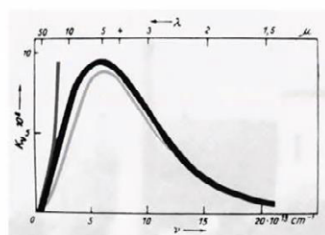
Upcoming bwHPC-courses

bwHPC offers a statewide training program aimed at both beginners and advanced users, including introductory courses on the use of bwHPC clusters, courses on programming languages and parallel programming, and introductions to scientific applications. The current course offerings and registration information can be found below and ⋯⫶ **here.**

bwHPC-courses

Niveau	Topic	Title	Time	Location	Registration
Advanced course	**Programming**	ONLINE COURSE: Modern C++ Software Design (Intermediate)	08.03.2022 11.03.2022	Uni Stuttgart	hlrs.de/training/2 022 03 08 cpp1
Basic course	**Introduction course**	Introduction to HPC Cluster bwUniCluster 2.0	22.03.2022	Online course	training.bwhpc.de /...64&client_ BWHPC
Basic course	**Parallel programming**	MATLAB on HPC	24.03.2022	Online course	training.bwhpc.de /...47&client_BWHPC
Advanced course	**Tools**	Iterative Linear Solvers and Parallelization	28.03.2022 01.04.2022	Uni Stuttgart	hlrs.de/training/2 022 03 28 iter s/
Basic course	**Introduction course**	Introductory Course: HPC and Data Management in Baden-Württemberg	07.04.2022	KIT Karlsruhe	https://indico.scc. kit.edu/event/2667/
Advanced course	**Introductory courses**	Advanced HPC and Data Management topics	13.04.2022	KIT Karlsruhe	https://indico.scc.kit.edu/ event/2666/
Advanced course	**Programming**	Modern C++ Software Design (Advanced)	03.05.2022 06.05.2022	Uni Stuttgart	hlrs.de/training/2 022 05 03 cpp2/
Advanced course	**Parallel programming**	ONLINE COURSE: Efficient Parallel Programming with GASPI)	20.06.2022 21.06.2022	Uni Stuttgart	hlrs.de/training/2022-06-20-gaspi/
Advanced course	**Programming**	Modern C++ Software Design (Intermediate)	21.06.2022 24.06.2022	Uni Stuttgart	hlrs.de/training/2 022 06 21 cpp3/
Advanced course	**Programming**	ONLINE COURSE: Node Level Performance Engineering	28.06.2022 01.07.2022	Uni Stuttgart	https://www.hlrs. de/training/2022/ NLP

Introducing the bwHPC Competence Center for Bioinformatics and Astrophysics

The competence center for Bioinformatics and Astrophysics (CCBinA) supports researchers in all aspects of high perfomance computing on the bwForCluster BinAC located in Tübingen. Fittingly, the server building in which the BinAC resides is right in the eyeshot of some biology research groups.

The competence center members themselves are working in the IT Center at the University of Tübingen and KIM (Communication, Information, Media) Center at the University of Konstanz.

Researchers can profit from the competence center staff's longstanding experience in bioinformatics and high performance cluster operations. The support offered by the team has many facets, which will be highlighted in the course of this article. One aspect is user training and documentation of the cluster and its features. Especially the training courses ran regularly by CC BinA members help novice users who are unfamiliar with Linux systems and HPC environments with their first steps on the BinAC cluster.

Before number crunching via compute jobs can take place on the cluster, researchers need a suitable software environment. Some software packages are already provided as enviroment modules, especially a plethora of compilers, libraries, and MPI implementations. This is usually sufficient for researches who write or compile their code themselves. But in many cases, especially in the bioinformatics field, researchers use software or ready to use pipelines written by other research groups and organisations.

Sometimes the software or pipeline is only available for a specific Linux distribution and cannot be run out of the box on the Red Hat operating system of BinAC. In this cases we can support the user by either porting the application to Red Hat or, if this is not feasible, build and test custom software containers for the user.

This is not the end of the support spectrum covered by CC BinA, as new issues emerge when running applications on several compute nodes or bigger datasets. These issues are often related to efficiency, resulting in inefficient use of the computing resources or even making the computation seemingly impossible, as limited resources like memory are not sufficient. Here the CC BinA members can support the researchers in to parallelize the workload more efficiently and use limited resources (e.g. memory) more efficiently. One example from the past would be reducing the memory consumption of an R Script by 50% by understanding the underlying memory management of R and suggesting subtle changes in the script, such that the researcher was able to run the analysis on the BinAC hardware.
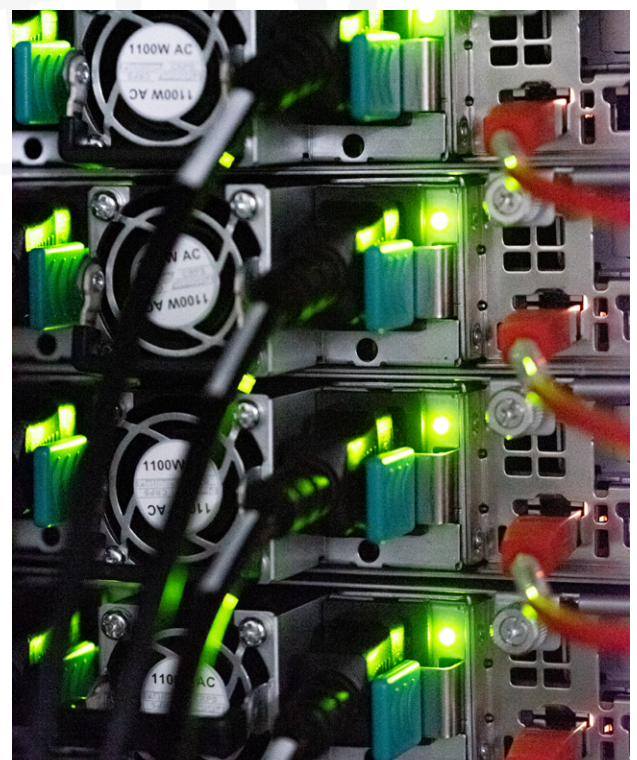
Server Room, Foto by Christoph Jäckle, University of Tübingen

Number crunching is a very important aspect of research, but data management and the data life cycle is becoming more and more important. Hence members of the CC BinA are working on automated annotation of technical metadata for research data, which can then be stored in research data repositories for later publication. This feature is developed with regard to Science Data Center BioDATEN.

As the BinAC reaches the end of its lifetime, the operators at IT Center in Tübigen are currently planning a new HPC system using newest available technologies. Beside the support acitivities depicted in the previous paragraphs, this will be the main task for us in 2022.

> Some interesting Numbers:
> ■ 593 registered users on BinAC
> ■ >241 publications from researchers using the BinAC
> ■ 10.000.000 compute Jobs ran on BinAC since November 2016
> ■ >1400 solved tickets since November 2016

Revised Registration Guide

We hear you.
In the past, we have repeatedly received messages that the wiki sometimes contains outdated and no longer completely correct information. After several years of operation and several clusters, this can happen over time. However, the wiki is intended to be a help to users when they get stuck or have access problems, not to raise more questions.
As some may have noticed, we have started to restructure the wiki and update information. Now we have achieved a first goal. The registration instructions have been largely unified and updated. Please feel free to give us feedback on this via the bwSupport portal. Please note that the wiki is still under reconstruction, only the registration is considered revised.

Invitation E-Science Tage 2023

We are very pleased to inform you that the **E-Science-Tage 2023** under the motto „Empower Your Research – Preserve Your Data" will be taking place from **1 to 3 March 2023** in Heidelberg.

Following the focus of the E-Science-Tage 2021 on the sharing of research data, the upcoming conference will focus on strengthening scientific research by promoting the sustainable storage and preservation of research data.

We cordially invite you to join us. Please be sure to save the date! More detailed information to follow.

We are looking forward to seeing you in Heidelberg in March 2023!

Your E-Science-Tage 2023 Organizing Team
Email: e-science-tage@uni-heidelberg.de
Website: https://e-science-tage.de/
Twitter: https://twitter.com/EsciTage
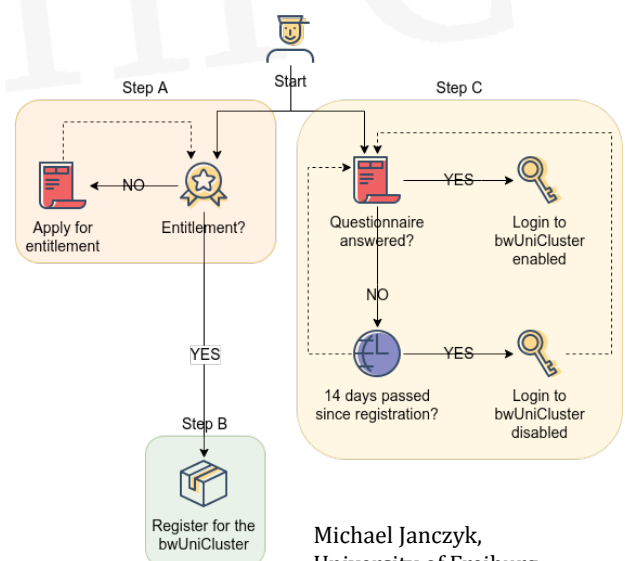
Michael Janczyk,
University of Freiburg

You can access the instructions at:
https://wiki.bwhpc.de/e/Registration

Invitation:
Matlab on HPC Web Seminar Call for Participation

The bwHPC-Training-Team at HLRS, University of Stuttgart is pleased to announce its web seminar for bwHPC users.

Web Seminar MATLAB on HPC
https://training.bwhpc.de/goto.php?target=crs_647&client_id=BWHPC

Thursday **March 24, 2022,**
 limited number of spots (35)

This MATLAB on HPC training is a course on software development with the MATLAB programming language. The focus of the training are the essential parallel programming principles, concepts, idioms, and best practices, which enable programmers to create professional, high-quality code. The course will give insight into the different aspects of parallelization, vectorization and optimization with MATLAB and will teach guidelines to develop mature, robust, maintainable, and efficient code. In addition, the course will give an introduction to the use of MATLAB on bwUniCluster 2.0, including the batch system, workspace, module files, visualization and interactive jobs.
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Learning Sequence:
- Parallel Computing with MATLAB
- Using MATLAB on bwUniCluster 2.0
- Digression: Use MATLAB in Jupyter Note books on bwUniCluster 2.0 (Live Demo)

After this course, participants will...
- understand the basic concept of parallel computing
- know about the limitations of parallel computing
- have gained knowledge about the types of parallel programming
- be able to properly write parallel code
- know about the parallelization, vectorization and optimization
- have a detailed understanding about the most important commands on the bwUniCluster 2.0
- gained knowledge how to user MATLAB in Jupyter Notebooks

Prerequisites:
- A general knowledge of programming as well as a background in MATLAB programming is useful for understanding this course. MATLAB should already be installed on the participants computer.

- The background of Linux as well as the most important concepts and tools of Linux should be known, e.g.
■ Shell and shell commands (→safe use of the command line),

Invitation: Matlab on HPC Web Seminar Call for Participation

■ secure shell,
■ the handling of files and scripts,
■ the structure of the system,
■ the user and rights management and
■ creating simple batch scripts with an editor like nano, vi or emacs.

If you still notice deficits in this respect, we refer you at this point to https://www.tuxcademy.org/product/lxes/.

- Experience with connecting to the bwUniCluster 2.0 as well as file systems, data transfer and using the batch system and environment module system on bwUniCluster 2.0, e.g., from participation in previous course „Introduction to HPC-Cluster-bwUniCluster 2.0" - https://training.bwhpc.de/goto.php?target=crs_664&client_id=BWHPC

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Date & Location:

Online Webex, HLRS, University of Stuttgart, Germany
- Online Kick Off: 2022,
  Thursday March 24, 09:00 – 10:30
- Self-Study Phase: 2022,
  Thursday March 24, 10:30 – 15:00
- Online Closing: 2022,
  Thursday March 24, 15:00 – 16:30

Webex-Invitation will be sent directly by e-mail to the registered participants.

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Registration and further information:
- bwHPC-Ilias (Learning Management System): https://training.bwhpc.de/goto.php?tar-get=crs_647&client_id=BWHPC

- bwUniCluster 2.0
■ Obtainment of bwUniCluster entitlement: https://training.bwhpc.de/goto.php?tar-get=pg_5102_311&client_id=BWHPC
■ Further information on bwHPC-Wiki: https://wiki.bwhpc.de/e/BwUniCluster_2.0_User_Access

Deadline for registration:
2022, Tuesday March 22, 09:00
Limited number of spots (35)

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Lecturer:
Darko Milakovic (HLRS)
- The course language is German but slides are in English.
- It is recommended to try the code examples yourself interactively by using your own computer with MATLAB already installed.
- With a successful registration for the course, the participants get access to the content on the bwHPC-Ilias
- The participants need to have access to the bwUniCluster 2.0, for this they need the bwUniCluster entitlement

Due to the limited number of free spots (35) early registration is recommended.

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Further upcoming courses 2022
that may be of interest for you:
- https://www.hlrs.de/training/
- https://training.bwhpc.de/goto.php?tar get=dcl_96_41&client_id=BWHPC

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You can not fit our course dates into your busy schedule? Please let us know.
We will offer further course dates if there will be more prospective attendees.

Invitation: Introduction to HPC-Cluster - Web Seminar Call for Participation

The **bwHPC-Training-Team at HLRS,** University of Stuttgart is pleased to announce its web seminar for bwHPC users.

Web Seminar Introduction to HPC-Cluster
- bwUniCluster 2.0
- Introduction to HPC-Cluster - bwUniCluster 2.0
- https://training.bwhpc.de/goto.php?target=crs_664&client_id=BWHPC - Tuesday **March 22, 2022, 09:00 – 12:00**, limited number of spots (35)

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Abstract:
High Performance Computing (HPC) means achieving high and highest computing performance. Special HPC clusters and supercomputers are used for this purpose. To achieve maximum performance, all the components involved must be planned and coordinated and operated with each other. The course will give insight into the need for supercomputers and teach the basic structure of a microprocessor and multicore processor (x86_64) as well as the different aspects of of shared memory CPU-nodes and distributed memory systems. In addition, the course will give an introduction of the bwUniCluster 2.0, including the connection, authentication, batch system, workspaces, module files, visualization, data transfer, file systems and interactive jobs.
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Agenda:
- Why HPC-Cluster / Cluster Computing?
- System Architecture
- Compute Nodes with Multiple Processors
- Coffee Break
- Cluster Basics
- Coffee Break
- Hands On/Live Demo on bwUniCluster 2.0 (1)
- Coffee Break
- Digression: Use Bash in Jupyter Notebooks on bwUniCluster 2.0 (Live Demo)

After this course, participants will...
- understand the benefits of HPC clusters
- know the basics about system architecture
- have gained knowledge about the difference of shared memory CPU-nodes and distributed memory systems
- be able to properly connect to the bwUniCluster 2.0
- know about the file systems, enviroment module system, data transfer on the bwUniCluster 2.0
- have a detailed understanding about the most important commands (of the batch system) on the bwUniCluster 2.0

Invitation: Introduction to HPC-Cluster - Web Seminar Call for Participation

Prerequisites:
- The background of Linux as well as the most important concepts and tools of Linux should be known, e.g.
■ Shell and shell commands (→safe use of the command line),
■ secure shell,
■ the handling of files and scripts,
■ the structure of the system,
■ the user and rights management and
■ creating simple batch scripts with an editor like nano, vi or emacs.
If you still notice deficits in this respect, we refer you at this point to https://www.tuxcademy.org/product/lxes/.
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Date & Location:
Online Webex, HLRS, University of Stuttgart, Germany
- Online Web-Seminar:
2022, Tuesday March 22, 09:00 – 12:00
Webex-Invitation will be sent directly by e-mail to the registered participants.

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Registration and further information:
- bwHPC-Ilias (Learning Management System): https://training.bwhpc.de/goto.php?target=crs_664&client_id=BWHPC
- bwUniCluster 2.0
■ Obtainment of bwUniCluster entitlement: https://training.bwhpc.de/goto.php?target=pg_5102_311&client_id=BWHPC
■ Further information on bwHPC-Wiki: https://wiki.bwhpc.de/e/BwUniCluster_2.0_User_Access

Deadline for registration:
2022, Monday March 21, 09:00
Limited number of spots (35)

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Lecturer:
Darko Milakovic (HLRS)
- The course language is German but slides are in English.
- It is recommended to try the code/command examples yourself interactively by using your own computer.
- With a successful registration for the course, the participants get access to the content on the bwHPC-Ilias
- The participants need to have access to the bwUniCluster 2.0, for this they need the bwUniCluster entitlement
  Due to the limited number of free spots (35) early registration is recommended.

Further upcoming courses 2022 that may be of interest for you:
- https://www.hlrs.de/training/
- https://training.bwhpc.de/goto.php?target=dcl_96_41&client_id=BWHPC

You can not fit our course dates into your busy schedule? Please let us know.
We will offer further course dates if there will be more prospective attendees.

Greetings from the bwHPC team

Here comes the sun,
and I say
It's all right.

THE BEATLES

For today we send you warm greetings from the bwHPC team and wish you a belated happy new year and a pleasant working time.

Imprint

The authors of the text contributions bear sole responsibility for content and referenced web pages.

The editorial staff uses gender-appropriate language. In individual cases there may be deviations for reasons of easier legibility. At this point we expressly point out that both the male and the female spelling are meant for the corresponding contributions.