



NEMO Cluster Location: University of Freiburg

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



We present our Competence Center for Structural and Systems Biology, Medical Science, Computational Humanities, and Soft Matter

The bwHPC Competence Center for Structural and Systems Biology, Medicine, Computational Humanities and Soft Matter supports researchers in High Performance Computing on the new bwForCluster Helix in Heidelberg and before that on the predecessor system bwFor Cluster MLS&WISO since 2015.

The statewide bwHPC competence center is coordinated by Heidelberg University Computing Center (URZ) and the University IT Mannheim (UNIT). It offers comprehensive support and an optimized software stack tailored to users with a wide range of research interests from biology to sociology.

The challenges of the competence center arise from the diversity of methods and data used by the various research communities. The use cases range from computational-intensive simulations to data-intensive computing and all require the provision of appropriate numerical software and libraries. Enabling easy access to specialized environments or the combined use of other state services such as SDS@HD, bwVisu and bwCloud are further tasks of the competence center. With the start of bwForCluster Helix the focus is on migration support and the provision of optimized software for the new hardware.

Currently the competence center supports about 700 active users. Usage documentation is maintained in the bwHPC Wiki. Users are mainly supported via support tickets, but also via face-to-face meetings in case of special requests. For more extensive and complicated problems, it is possible to set up a Tiger Team, a dedicated collaboration to solve technical issues and research questions. In the past, this invol-

ved for example optimization of data access and provision of a tool chain for cryo-electron microscopy or developing a workflow for imagine analysis of old Italian texts on the cluster. Each year the competence center welcomes about 100-150 new users. Many are using an HPC system for the first time. HPC beginners or more experienced users new to the system can join an introductory online course on the bwHPC training platform which is permanently open for registration.

You can reach the bwHPC Competence Center either via the bwHPC support portal:
<https://www.bwhpc.de/supportportal>

New HPC-System „bwForCluster Helix“ in Heidelberg Now in Operation

The new High Performance Computing (HPC) system „bwForCluster Helix“ went into operation in August 2022 as a state service for all researchers at Baden Württemberg universities, colleges and research institutes in the bwIDM network.

Helix is the successor system to „bwForCluster MLS&WISO“ and is operated by the Heidelberg University Computing Centre (URZ). The users of „bwForCluster MLS&WISO“ have started working with Helix and new users are welcome.

In order to make the transition to Helix as smooth as possible for researchers and to avoid interruptions to ongoing projects, „bwForCluster MLS&WISO“ continues to operate in parallel until 23 September 2022.

The compute nodes of bwForCluster Helix are equipped with AMD EPYC Milan processors and NVIDIA Ampere GPUs making Helix significantly more powerful than its predecessor. On Helix, researchers will be able to work across systems due to a direct connection to the SDS@hd state service for the storage of research data, a service also operated at the URZ. This makes generating, analyzing and storing large amounts of research data particularly efficient. Helix is to be used primarily for data- and compute-intensive research in the life sciences, natural sciences and computational humanities.

How the compute nodes are equipped in detail and how the system can be used is described in the bwHPC Wiki. User support is provided by the bwHPC competence center for Structural and Systems Biology, Medical Science, Computational Humanities, and Soft Matter which is presented in a separate article.

Service Description:

<https://www.urz.uni-heidelberg.de/de/service-katalog/hochleistungsrechnen/bwforcluster-helix>

bwForCluster Helix in the bwHPC Wiki:

<https://wiki.bwhpc.de/e/Helix>



Helix hardware at a glance

- ca. 20,000 AMD EPYC Milan processor cores
- ca. 100 TB of main memory
- ca. 200 NVIDIA Ampere Tensor Core GPUs (A100 and A40)
- Non-blocking NVIDIA Mellanox InfiniBand HDR (at least 100 GBit/s per compute node)
- High performance storage with a parallel IBM Spectrum Scale file system: total capacity of ca. 11 PB, flash storage of ca. 800 TB

Flashback: ISC Conference 2022 bwHPC summary of an exciting exhibition at ISC 2022

The ISC exhibition is the International Supercomputing Conference and Europe's leading conference and exhibition for High Performance Computing, Networking, Storage, High Performance Data Analytics and AI/Machine Learning. ISC is dedicated to the technological development of High Performance Computing (HPC) and its application in scientific fields as well as its application in commercial environments. ISC also represents the largest European event for exchange between HPC vendors, universities and research organizations.

This year, around 100 national and international exhibitors presented their products and services at the ISC 2022 conference, which was held in Hamburg, Germany, from May 30 to June 01, 2022, and was attended by more than 3,000 participants. The range of offerings at the International Supercomputing Conference in Hamburg included innovative architectures such as GPGPU and accelerator-based systems, multicore and manycore systems, as well as networking technologies and applications or data management and storage systems. In addition, numerous supercomputing topics, innovations and applications were discussed and presented at ISC.

After a two-year break due to the pandemic, the bwHPC project was again represented at Europe's largest HPC forum, ISC High Performance 2022, with an information booth on the state-wide bwHPC alliance.

The bwHPC booth team welcomed more than 120 ISC visitors and had interesting discussions about the bwHPC-S5 project (Scientific Simulation and Storage Support Services). A wide range of mini-presentations rounded out the booth activities. In the process, the bwHPC-S5 project successfully expanded the visibility of bwHPC on a national and international level and established new contacts with a variety of internationally recognized centers.

It is planned that we will participate in the ISC again next year. ISC'23 will take place in Hamburg on May 21-25.





Feedback: bwHPC User Survey 2022

We as the bwHPC team want to say **Thank you** for your feedback!

Your sincere and open opinion is important to us. Only in this way, we can fulfill our ambition to be able to advise you as a user individually and competently. We thank you for your suggestions and comments, because they help us to improve our service and support on a daily basis. Given

that the survey revealed a great need for support and assistance, we would like to refer you to the bwHPC support page by presenting three support possibilities.

Survey participants: 372

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 I here.

bwHPC-courses



Niveau	Topic	Title	Time	Location	Registration
Basic course	Introduction courses	Introductory Course 2022/10/13: HPC and Data Mngt. in Baden-Württemberg	13.10.22	ONLINE COURSE	https://indico.scc.kit.edu/event/3049/
Advanced course	Simulation	CFD with OpenFOAM®	17.10.22 - 21.10.22	Uni Stuttgart	https://www.hlrs.de/training/2022/OF1/
Advanced course	Introduction courses	Intermediate Course 2022/10/19: Advanced HPC and Data Management topics	19.10.22	ONLINE COURSE	https://indico.scc.kit.edu/event/3050/
Advanced course	Parallel programming	Introduction to GPU Programming using CUDA	14.11.22 - 17.11.22	Uni Stuttgart	https://www.hlrs.de/training/2022/CUDA
Advanced course	Programming	Modern C++ Software Design (Advanced)	22.11.22 - 25.11.22	Uni Stuttgart	http://www.hlrs.de/training/2022/_CPP4
Advanced course	Programming	ONLINE COURSE: Fortran for Scientific Computing	05.12.22 - 09.12.22	Uni Stuttgart	https://www.hlrs.de/training/2022/FTN3
Basic course	Machine Learning	From Machine Learning to Deep Learning: a concise introduction	12.12.22 - 16.12.22	Uni Stuttgart	https://www.hlrs.de/training/2022/dl-hlrs

Save the date: bwHPC Symposium 2022

We invite you to participate in the upcoming **8th bwHPC Symposium on November 28th, 2022**. The conference will take place online and focuses on the presentation of scientific projects and success stories carried out with the help of bwHPC high performance computing as well as the BaWü data federation. The event offers a unique opportunity to engage in an active dialog between the scientists, operators of the bwHPC services, and members of the bwHPC-S5 support centers.



Deadline for abstracts:

Monday, November 14, 2022

Deadline for registration:

Sunday, November 13, 2022



Registration

Registration for this event is currently open.
<https://indico.scc.kit.edu/event/2708/registrations/454/>



The call for abstracts is open

You can submit an abstract for reviewing.
<https://indico.scc.kit.edu/login/?next=%2Fevent%2F2708%2Fabstracts%2F%23submit-abstract>



Starts Monday,
November 28, 2022, at 09:00 am
Ends Monday,
November 28, 2022, 08:00 pm
Europe/Berlin



Zoom Online Event

For more information:

visit 8th bwHPC Symposium
<https://indico.scc.kit.edu/event/2708/>



E-Science Tage 2023: Call for Contributions

We are pleased to announce a Call for Contributions for 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.

The conference will be dedicated to the slogan „Empower Your Research - Preserve Your Data“, but the thematic focus of contributions does not have to be limited exclusively to this. Example subject areas include:

- Data archiving, reproducibility and reusability
- Data publication and Open Science
- Data formats and standards
- Data law, data protection and data security
- Quality assurance
- Specific and generic RDM tools
- Institutional approaches

Possible contribution formats include presentations, posters, Lightning Talks and workshops.

The detailed call for contributions with information about submission can be found at <https://e-science-tage.de/de/CFC2023>. We have compiled more information about the event formats as well as general information about the E-Science-Tage at <https://e-science-tage.de>.

We are looking forward to your contributions.

Best regards,

Your E-Science-Tage Organizational Team

Email: e-science-tage@uni-heidelberg.de

Website: <https://e-science-tage.de/>

Twitter: <https://twitter.com/EsCiTage>

Rising Energy costs

You are all aware of the rising energy costs and you are certainly careful to economize your energy consumption at home.

But are you aware that computing power also consumes energy?

An average compute job running on just a single node for one day can easily consume 10 kWh or even more.

That translates roughly to one of the following activities:

- toasting about 1330 slices of toast in a toaster
- continuously blow-drying your hair for about 10 hours
- actively working on a laptop for about 500 hours
- brewing 700 cups of coffee
- cooking 40 dinners

Besides energy costs, even this single job alone will also contribute to climate change by adding around 5 kg of CO₂ to the atmosphere which is roughly equivalent to driving a distance of 30 km by car.

You get the point: Please always keep this in mind when submitting tens or even hundreds of jobs to the queue, just like you do when switching on your electrical devices at home. Also, please always think carefully about how many resources your jobs really need and whether your application really benefits from allocating more cores for the jobs. Application speedup is often limited and does not scale linearly with the number of dedicated cores. But energy consumption usually does ...



**Using as many resources as possible does not make a power user. Using them wisely does.
If in doubt, just ask.**

Greetings from the bwHPC team



„If a year was tucked inside a clock,
then Autumn would be
the magic hour.“ —Victoria Erickson

For today we send you warm greetings from the bwHPC team and wish you a pleasant and good start after the relaxing summer break.

Imprint

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Steinbuch Center for Computing
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Communication and Information
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E-mail: office@bwHPC.de

Editorial Office
Isa Karabulut, University of Ulm
Phone: +49 (0)731 50 - 22483
Fax: +49 (0)731 50 - 22471
E-mail: isa.karabulut@uni-ulm.de

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Department of Media



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