News

bwUniCluster 2.0

bwHPC Newsletter

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Dear bwHPC users,

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

bwHPC team

Feedback: bwHPC user Survey

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 highlight three support options below.
Survey participants: 370
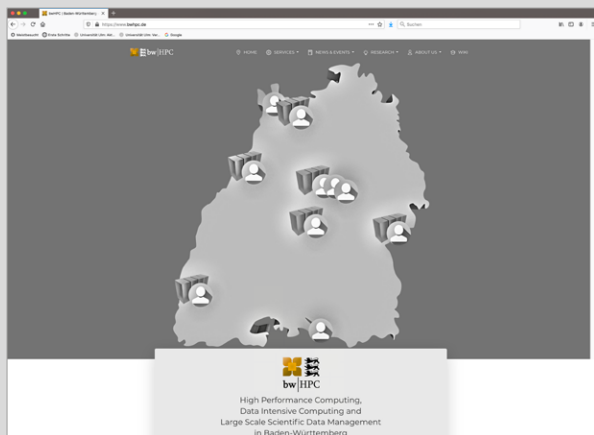
The project website and the associated bwHPC wiki are used extensively for information about access to all clusters in Baden-Württemberg (bwUniCluster, bwForCluster, and higher performance tiers), „best practices" in handling systems and software packages, the processes involved in applying for computing projects, documentation of the various hardware components, explanations of security measures, and announcements of planned maintenance dates and any malfunctions. In order to provide a quick overview of the status of all cluster and storage systems, operationally relevant information (e.g. announcements, current disruptions, scientific software offerings) is automatically extracted from the other basic services, summarized and presented collectively on the project website. We are continuously working on a better clarity of the website and the associated ⋯⇥ **bwHPC wiki.**

Call for Tiger Team Support Application
With this call, we would like to draw the attention of all users of the bwHPC systems bwForCluster/bwUniCluster once again to our special support offer ‚Tiger Team Support'. A tiger team is initiated by an HPC competence center for more extensive support and optimization measures in order to work on a specific task together with the users, for example porting an application to a bwHPC cluster, optimizing batch scripts or the parallelization of program parts. Workflows and data management on the HPC and storage systems can also be investigated and improved as part of a tiger team.

A more detailed description of the **support service** can be found on the ⋯⇥ **website**:
There you can request Tigerteam support for your demands via an online form.
Alternatively, you can also contact your bwHPC competence center via the support addresses of the cluster and storage systems and informally ask for Tigerteam support.
The bwHPC competence centers look forward to interesting tasks and to working with you.

Workshops

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	**Simulation**	CFD with OpenFOAM®	20.09.2021-24.09.2021	Uni Stuttgart	https://www.hlrs.de/events
Advanced course	**Pre-& Postprocessing**	Scientific Visualization	30.09.2021-01.10.2021	Uni Stuttgart	https://www.hlrs.de/events
Advanced course	**Parallel programming**	ONLINE COURSE: Parallel Programming Workshop (MPI, OpenMP and Advanced Topics)	11.10.2021-15.10.2021	Uni Stuttgart	https://www.hlrs.de/events
Basic course	**Introductory courses**	BinAC training	12.10.2021-13.10.2021	Online course	uni-tuebingen.de/e...inac-schulung-2021
Advanced course	**Parallel programming**	ONLINE COURSE: ChEESE Advanced Training on HPC for Computational Seismology	19.10.2021-21.10.2021	Uni Stuttgart	https://www.hlrs.de/events
Basic course	**Introductory courses**	Introductory Course: HPC and Data Management in Baden-Württemberg	21.10.2021	KIT Karlsruhe	https://indico.scc.kit.edu/category/17
Advanced course	**Introductory courses**	Advanced HPC and Data Management topics	27.10.2021	KIT Karlsruhe	https://indico.scc.kit.edu/category/17
Advanced course	**Programming**	Modern C++ Software Design (Advanced)	23.11.2021 - 26.11.2021	Uni Stuttgart	https://www.hlrs.de/events
Advanced course	**Programming**	Fortran for Scientific Computing	06.12.2021 - 10.12.2021	Uni Stuttgart	hlrs.de/training/2021-12-06-ftn2
Advanced course	**Programming**	Modern C++ Software Design (Intermediate)	08.03.2022 - 11.03.2022	Uni Stuttgart	https://www.hlrs.de/events
Advanced course	**Programming**	Modern C++ Software Design (Advanced)	03.05.2022 - 06.05.2022	Uni Stuttgart	https://www.hlrs.de/events
Advanced course	**Programming**	Modern C++ Software Design (Advanced)	05.07.2022 - 08.07.2022	Uni Stuttgart	https://www.hlrs.de/events

Online Courses

To ensure constant, location-independent access to information, we are building online courses for self-study on our training platform training.bwhpc.de.

„The Introduction to bwHPC" course offers first steps for beginners (login, data transfer) and explains how to use the batch system.

The introductory course „Linux Basics" provides concise and precise instructions on how to use Linux on the bwHPC clusters.
The results of the survey support us in prioritizing the development of new e-learning courses.

Click here for the ⋯⋯⟩ **e-learning courses**

News Item E-Science-Tage 2021

„Share Your Research Data" was the theme of the 3rd E-Science-Tage, held online for the first time on March 4-5, 2021. In a wide range of individual events, more than 600 participants discussed the benefits and risks that the open exchange of research data can bring for scientific endeavors, for example regarding transparency, research quality and general knowledge advancement. Concepts and strategies for the infrastructure required for the sharing of research data were presented and discussed. Even in a virtual setting, the E-Science-Tage offered ample opportunity for exchanging new ideas and stimuli from the world of research data management (RDM). Minister of Science Theresia Bauer, Prof. Dr. Dr. h.c. Bernhard Eitel, Rector of Heidelberg University and Prof. Dr. Vincent Heuveline, Director of the Heidelberg University Computing Centre (URZ) opened the digital E-Science-Tage. "There are many possibilities associated with the sharing of research data: It spurs discourse, increases knowledge & ensures scientific quality," commented Minister Bauer on Twitter after the virtual kickoff. The rector emphasized the importance of research data management for knowledge advancement: „Research data is a resource which deserves special attention!"

Over the two-day event, participants were able to attend presentations in virtual conference rooms, join workshops and network via the digital conferencing platform. Other program highlights were the keynotes by Prof. Dr. York Sure-Vetter on the National Research Data Infrastructure (NFDI) and by Prof. Dr. Martin Wikelski on "Movebank – The Database behind the Internet of Animals". The final panel discussion between RDM experts grappled with the question of whether sharing research data is merely ideological wishful thinking or an inevitable necessity. At the conclusion of the conference, prizes were awarded for the three best poster contributions.
The event was funded by the Ministry of Science, Research and the Arts Baden Württemberg and was organized by the Heidelberg University Computing Centre service area Future IT - Research & Education (FIRE) team in cooperation with project partners at the University of Konstanz and the Karlsruhe Institute of Technology.
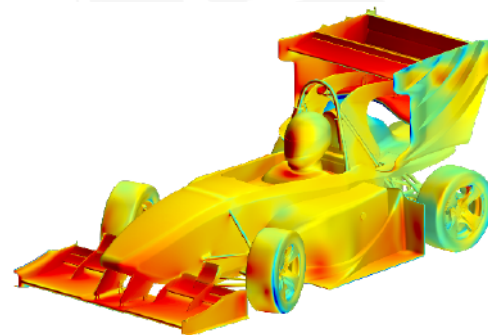
Introducing the Competence Center for Engineering

The competence center for engineering sciences (Competence Center ENG, or CC- ENG) has one of the largest community of students and researchers in Baden-Württemberg which makes use of the introductory-level of supercomputing. The CC-ENG and its customers gain benefit from the strong engineering communities at all Universities of Baden-Württemberg as well as at the Universities of Applied Sciences and the cooperation of their computing centers within the bwHPC-S5-projects.

While the University of Stuttgart operates at the highest supercomputing level in Europe, the supercomputer of choice for many engineers, students and PhD-students in Baden-Württemberg is the bw-Uni-Cluster (shortly UC2), which is located at the Steinbuch Centre for Computing (SCC) of the Karlsruhe Institute of Technology. Currently, it has more than 28800 computing cores as well as 136 GPUs which are available for the engineering community. Here, students as well as postdoctoral scientists can perform their first projects discovering the power of supercomputing as a booster for their research problems. The switch from a single desktop computer or workstation to the bwUniCluster 2.0 is supported with courses (one to three days duration which is adapted to the level of the users) given in cooperation with other competence centers. At these courses, students and researchers get an overview of choosing the suitable queue and of submitting parallel jobs for their applications. Their first steps in supercomputing are supported further by individual help from the CC-ENG team members.

A further duty of the CC-ENG is the installation and support of specific parallel software and post-processing tools targeting the solution of engineering problems; both commercial and open-source software is supported. Widely used software packages are those for solving problems in Computational Fluid Mechanics (CFD) and Numerical Heat Transfer. An interesting example is the Formula Student project at the University of Applied Sciences in Esslingen. A team of around 40 students from mechanical engineering, automotive engineering, engineering management and media students develop a single seated racecar for a period of twelve months. The students used the bwUniCluster to optimize its

aerodynamics. Some results of the CFD simulations of the Formula Student team of Esslingen (Rennstall Esslingen) showing the pressure distribution on the car are shown in the figures.

Pressure distribution at the surface of the race car (isoview)
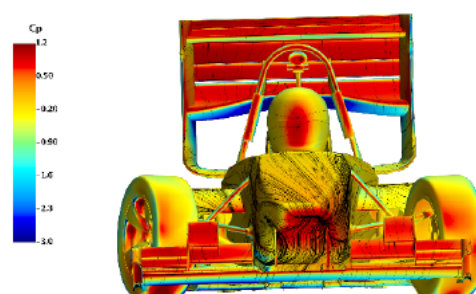
Pressure distribution and streamlines at the front of the race car

Introducing the Competence Center for Engineering

The CC-ENG team also supports users which have more complex requirements or which want to use a specific combination of software packages. The latter is often the case when engineers seek for the solution of multiphysics problems, as e.g. the computation of two-phase problems (e.g. drying and thermal procession of biomass particles), of fluid-structure interactions (e.g. computing the stability of bridges or turbine rotor blades on wind gusts), or of flows with chemical reactions (e.g. in combustion of e-fuels). In such cases the efficient use of supercomputing requires a certain choice of parameters that is often assisted by the so-called „tiger-teams". These teams combine different experts of different computing centers for obtaining the desired engineering results through efficient parallel computations. In this case, the users are guided step-by-step until the final target is fulfilled. The achieved solution is then distributed to all computing centers and all user communities so that it can be reproduced on demand and further improved.

The CC-ENG team will continue their activities in supporting the engineering community with up-to-date parallel software and advanced supercomputing solutions so that the state of Baden-Württemberg will keep its leading position in the education and research in the field of engineering within Germany and Europe.

The Stellardo racing car at the start (2019)

Written by Jordan Denev (KIT)

DFG peer review of bwForClusters BinAC 2 & NEMO 2

Since their commissioning in 2016, the two high-performance computers BinAC[1] in Tübingen and NEMO[2] in Freiburg have been supplying researchers from the fields of astrophysics, bioinformatics, geosciences (BINAC) and neurosciences, elementary particle physics, microsystems technology, and materials sciences (NEMO). Further support with modern computing power is assured for the future, as the German Research Foundation (DFG) has approved the applications for the follow-up systems BinAC 2 and NEMO 2.

After an upstream positive evaluation by the Ministry of Science, Research and the Arts of the State of Baden-Württemberg, the applications for the bwForClusters BinAC 2 and NEMO 2 were submitted to the German Research Foundation (DFG) for review at the end of 2020. In December, a virtual review meeting took place at which, in addition to other projects from Baden-Württemberg, questions from the experts about the new systems were answered. Formal approval then followed in April 2021. Both high-performance computing systems, BinAC 2 and NEMO 2, will be fully funded with an investment volume of over €4 million each. These amounts include contributions from user groups, the universities, the state, as well as funding from the DFG under Article 91b of the German Basic Law.

At both the Freiburg and Tübingen sites, the respective teams are intensively engaged in the preparations for the tenders for the HPC systems. The goal is to identify the most powerful CPU and GPU configurations possible in order to be able to provide the best possible configuration for researchers from the respective scientific fields, which will also represent an attractive working platform over the planned operating period of five years.

In addition, a special focus is on improved support for researchers in the management of data. Modern high-performance computers should have a high-performance workspace for active work on „hot" research data. The industry is currently in the middle of a paradigm shift from spinning hard disks (slow but cheap) to flash storage (fast but even more expensive). While permanent storage of all research data on flash memory would be desirable, it is not economically feasible at this time. Concepts are therefore being actively worked on that would allow „lukewarm" research data to be stored on less expensive storage systems, bridging the gap between active processing and archiving. Here, the distributed storage system „Storage for Science" (bwSFS[3]) will play a special role. At the same time, integration with research data infrastructures such as Biodata[4], DataPLANT[5] and GHGA[6] is the subject of current work.

Technical and organizational challenges still need to be overcome at both the Tübingen and Freiburg sites. Nevertheless, the bwHPC teams are confident that they will be able to put the two high-performance computing systems into operation in the summer of 2022.

Written by Jens Krüger,
University of Tübingen,
and Bernd Wiebelt,
University of Freiburg

[1] https://www.binac.uni-tuebingen.de/
[2] https://www.nemo.uni-freiburg.de/
[3] https://rdmg.uni-freiburg.de/posts/bwsfs/
[4] https://portal.biodaten.info/
[5] https://nfdi4plants.de/
[6] https://ghga.dkfz.de/

DFG peer review of IT service project bwHPC-S5 Phase 2

In 2020 the bwHPC consortium drew up the Phase 2 of the state-wide IT service project bwHPC-S5 ‚Scientific Simulation and Storage Support Services' for high-performance computing, data intensive computing and large scale scientific data management in the State of Baden-Württemberg, Germany, establishing an integrated statewide computing and data storage infrastructure, increasing its efficiency and effectiveness through first-class user support, and furthering integrated view of services for users. The project plan has been positively reviewed by the DFG. Given the approval by Ministry of Science, Research and the Arts of the State of Baden-Württemberg for fully funding, bwHPC-S5 which started at Juli 2018 (as Phase 1) transitioned to Phase 2 on April 01, 2021. Phase 2 will run until June 30, 2023.

On April 22, 2021, the full project plan as well as the tasks for the next 3 months were presented to the colleagues of the science data centers (SDCs) and to the associates and members of bwHPC. The project team will continue its work started in bwHPC-S5 Phase 1 - e.g. user support of the HPC cluster and data facilities, maintaining software and services, teaching - but will also address more in detail the integration of HPC and (large scale) research data management and the required services for such an integration.

Written by Robert Barthel,
Project Management Office

Invitation:
bwHPC Symposium 2021

We invite you to participate in the upcoming **7th bwHPC Symposium on November 8th, 2021**. 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, October 25, 2021
Deadline for registration:
Monday, October 25, 2021

Registration
Registration for this event is currently open.
https://indico.scc.kit.edu/event/2399/
registrations/362

The call for abstracts is open
You can submit an abstract for reviewing.
https://indico.scc.kit.edu/event/2399/
abstracts

Starts Monday,
November 08, 2021, at 08:30 am
Ends Monday,
November 08, 2021, at 06:30 pm
Europe/Berlin

Ulm University
Zoom Online Event

For more information, visit:
https://indico.scc.kit.edu/event/2399

Greetings from the bwHPC team

Autumn is a second spring
when every leaf is a flower.

Albert Camus

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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At this point we expressly point out that both the male and the
female spelling are meant for the corresponding contributions.