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bw|HPC

News

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Flashback: 6th bwHPC Symposium 2019

Science meets High Performance Computing

On September 30, 2019, the 6th bwHPC Symposium took place at Karlsruhe Institute of Technology (KIT).

The opening speech was given by Dr. R. Dorn (Ministry of Science, Research and the Arts Baden-Württemberg, MWK) and two of the directors of the Steinbuch Centre for Computing, Prof. Dr. M. Frank and Prof. Dr. B. Neumair. Afterwards, Dr. R. Barthel, one of the bwHPC-S5 project managers, briefly presented the current achievements in bwHPC and the support project bwHPC-S5, which bridges science with high performance computing (HPC), data intensive computing (DIC) and large scale scientific data management (LS^2DM).

In the following, renowned scientists from various research fields, ranging from engineering over chemistry, neurosciences, bioinformatics and astrophysics to geosciences, presented their scientific projects and how those benefit from the bwHPC infrastructure and bwHPC-S5 services. During poster sessions and coffee breaks, the participants did discuss the poster (+20) covering bwHPC services as well as specific scientific results that had been achieved with the support thereof.

Flashback: 6th bwHPC Symposium 2019

Photo by Simon Raffeiner/KIT

The 6th bwHPC symposium has once again achieved its goal as an event of active exchange between HPC services and research, thereby bridging the gap between services providers and the scientific communities.

The upcoming 7th bwHPC Symposium 2020 will take place at Ulm University.

Written by Marion Moser/Ulm University

Upcoming bwHPC Courses

Level	Topic	Title	Begin	End	Location
Basic Course	Introduction	Introduction to bwHPC for Bioinformatics	18.12. 2019	18.12. 2019	University Konstanz Registration by email
Advanced Course	Parallel Programming	Introduction to Hybrid Programming in HPC	27.01. 2020	28.01. 2020	University Stuttgart hlrs.de/training/2020-01-27-hy-s
Basic Course	Introduction (in German only)	Einführungsveranstaltung bwHPC-S5	05.02. 2020	05.02. 2020	University Konstanz Registration by email
Special Course	Tools (in German only)	Linux Tutorial für bwHPC-Anwender	19.02. 2020	19.02. 2020	University Konstanz Registration by email
Advanced Course	Programming	Intermediate C++ with Focus on Software Engineering	03.03. 2020	06.03. 2020	University Stuttgart hlrs.de/training/2020-03-03-cpp1
Special Course	HPC Utilization (in German only)	Paralleles Arbeiten auf bwHPC-Systemen	04.03. 2020	04.03. 2020	University Konstanz Registration by email
Advanced Course	Simulation	CFD with OpenFOAM	16.03. 2020	20.03. 2020	University Stuttgart hlrs.de/training/2020-03-16-of1
Advanced Course	Tools	Iterative Linear Solvers and Parallelization	23.03. 2020	27.03. 2020	University Stuttgart hlrs.de/training/2020-03-23-iter-s

Announcements: bwHPC Webinars & bwHPC User Survey

Announcement:
bwHPC Webinars

In 2020 we will invite you to a series of webinars with bwHPC experts. The webinars will focus on special issues in a variety of topics such as parallel programming, Linux, introduction to the bwHPC clusters and scientific applications. In January 2020 we will start with a webinar about the usage of MATLAB on bwUniCluster.

Contact: training@bwhpc.de

Written by Bärbel Große-Wöhrmann /University Stuttgart

Announcement:
bwHPC User Survey

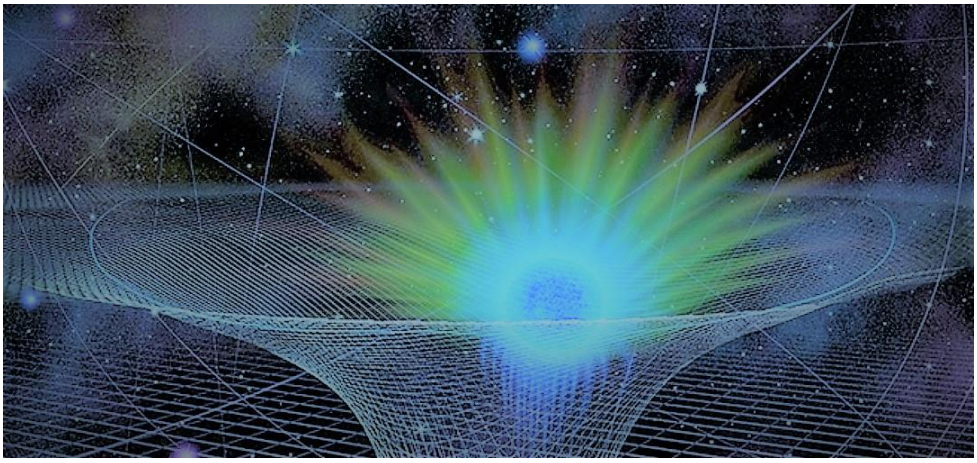
In order to continuously improve our services, we will conduct a user survey in January of 2020 again. This annual user survey will help us to better understand your current and future needs, identify potential for improvements to better meet your requirements and track key performance indicators. We'd also like to take the chance to thank you for your fantastic contributions to the bwHPC User Survey 2019. We have received 343 responses which we all have taken very seriously. We are looking forward to your feedback in the upcoming survey.

Written by Marion Moser/Ulm University

We present our Competence Center Geosciences

"The Geosciences competence center is one of the seven competence centers of the bwHPC initiative in Baden-Württemberg for HPC, DIC and LS^{2}DM."

It offers individual support for researchers in the geosciences when using bwForClusters such as BinAC. The centers, which are to be understood as organizational service units, link the scientific fields with the HPC cluster systems and support you in solving your subject-specific problems with regard to the implementation of high performance computing (HPC), data-intensive computing (DIC) and modern research data management. We also offer help with a change, e.g. from an entry-level cluster (bwUnicluster) to a bwForCluster corresponding to your discipline or to a higher HPC level of the performance pyramid, such as the ForHLR or the supercomputer at the HLRS. At the Geoscience Competence Center, IT experts and trained geoscientists advise you on your computing projects. Depending on your problem, it is also possible to set up a cross-site team of experts (TigerTeam) to address more complex scientific problems.



We present our Competence Center Geosciences

Due to the close cooperation and regular exchange between the bwHPC competence centers, interdisciplinary topics are also supported, as is the case with the CAMPOS Collaborative Research Centre at the University of Tübingen.
Information and training events are also planned and offered.
The Institute of Physics and Meteorology at the University of Hohenheim, for example, also offers non-Hohenheim geoscience students and researchers from Baden-Württemberg the opportunity to take part in a two-semester course in which knowledge and handling of the WRF model (numerical weather forecasting system) is imparted and this is applied in practice on high-performance computers.
In addition to supporting the efficient and sustainable use of the HPC systems, the Competence Center can also help you to find the right contact person for questions relating to research data management, e.g. data management plans, repositories, licenses, cost planning or similar.

You can reach the Competence Center Geoscience, as well as the other centers, either via the support system (https://bw-support.scc.kit.edu), where you can select the corresponding Competence Center in the "assign to" selection field or you can contact the spokespersons of the competence centers brigitte.wellenkamp@uni-hohenheim.de and jens.krueger@uni-tuebingen.de in person.

Written by Brigitte Wellenkamp/University of Hohenheim and Jens Krüger/University of Tübingen

Flashback: Gaussian Workshop 2019

The quantum chemistry program Gaussian offers extensive possibilities to calculate and examine chemical and physical properties of molecules and their chemical reactions.

The software is popular both in university research and teaching due to it's ease of use when tackling complex scientific problems. Furthermore the flexibility of the input, the multitude of available methods and approximations as well as the associated visualization program GaussView are essential elements for the success of the software.

In cooperation with the kiz and bwHPC, the comprehensive functionality of Gaussian and GaussView was presented to an international audience in a successful workshop that took place in the week from the 7th till 11th of October 2019 at the University of Ulm.

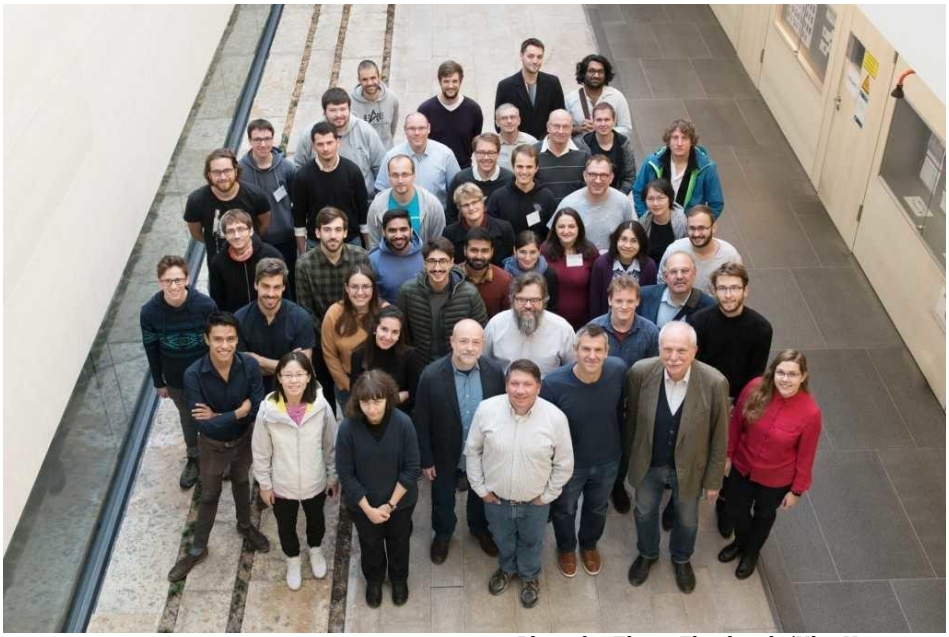


Photo by Elvira Eberhardt/Ulm University

Flashback: Gaussian Workshop 2019

The lectures and accompanying compute tutorials were supervised by six instructors with specific expertise in diverse areas of quantum chemistry. Overall 41 participants, 16 being from Baden-Württemberg, were able to gain in-depth knowledge into solving quantum chemical problems.
Besides technical aspects about how to use the software, great emphasis was put on teaching related quantum chemical knowledge.

Beyond the workshop itself the licenses for Gaussian and GaussView have been prolonged in the course of purchasing software for the next bwHPC compute cluster JUSTUS II. The software will be available to all users of the cluster within the next five years. The efficient use of the software is supplemented by a hardware accelerated remote visualization solution. This allows all bwHPC users to monitor their simulations and analyze their results without having to copy large amounts of data.

Looking back

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Steinbuch Center for Computing
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Ulm University
E-mail: office@bwHPC.de

Editorial Office & Layout:
Marion Moser, Ulm University
Phone: +49 (0)731 50-22483
Fax: +49 (0)731 50-22471
E-mail: marion.moser@uni-ulm.de

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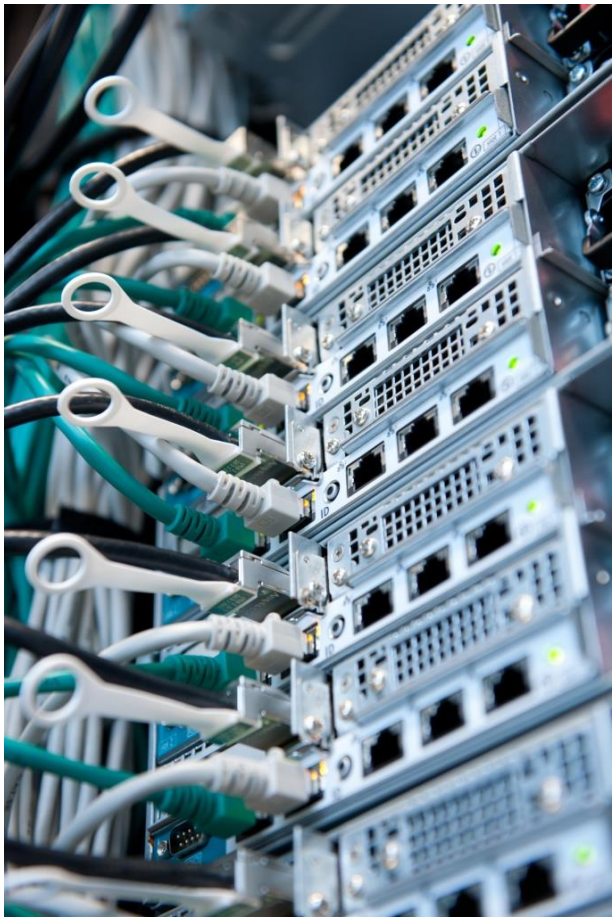

Photo by Elvira Eberhardt/Ulm University

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.

For further information please visit www.bwhpc.de