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IT Security Incident

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KIT introduces centralized 2-factor authentication for its HPC systems

In mid-May, a large number of HPC systems worldwide were affected by an IT security incident. The two high-performance computers ForHLR II (Tier-2) and bwUniCluster 2.0 (Tier-3) at KIT were put back into operation in mid-June. During the first out of three phases of the recommissioning process coordinated with the other operators in the federal state of Baden-Wuerttemberg, the use of SSH keys was no longer possible.

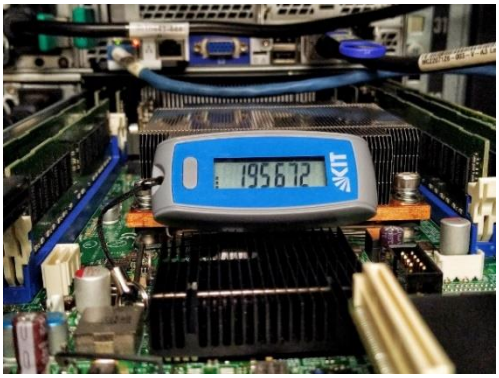

Photo by Simon Raffeiner/KIT

This caused severe restrictions for the scientific communities, especially on the Tier-2 system, since the HPC systems could no longer be integrated into automated scientific workflows.

Within just a few weeks, the Steinbuch Centre for Computing has successfully introduced a centrally managed 2-factor authentication (2FA) for all HPC systems using time-based one-time passwords (TOTP). So-called hardware or software tokens can be used to generate the one-time passwords. A wide range of software token solutions, including apps for mobile devices, is available. Registration and management of the tokens is handled by the web portal of the federal identity management system bwIDM.

In combination with the 2FA, the use of SSH keys is now possible again. These keys must also be managed via bwIDM. There are two types of SSH keys: those for interactive use and those for workflow automation (so-called “command keys”). SSH keys registered for interactive use allow the execution of any commands and require additional authentication with a time-based one-time password as a second factor. The second factor has to be entered once per hour at maximum. Command keys can be used without 2FA and thus

IT Security Incident

in an automated fashion. However, they must be restricted to a single command and have to be cleared by the HPC operations team.

Other operators from the bwHPC project are planning to introduce 2-factor authentication based on the new components developed for bwIDM. The source code is available to interested parties under an open source license.

Further information on 2-factor authentication for the HPC systems can be found in the user documentations for ForHLR II and bwUniCluster 2.0.

KIT führt zentrale 2-Faktor-Authentifizierung für HPC-Systeme ein

Mitte Mai wurde ein IT-Sicherheitsvorfall bekannt der eine Vielzahl von HPC-Systemen weltweit betraf. Auch der ForHLR II und der bwUniCluster 2.0 mussten vom Netz getrennt werden und konnten erst Mitte Juni wieder in Betrieb gehen. In der ersten abgestimmten Phase der Wiederinbetriebnahme war u.a. die Verwendung von SSH-Keys unterbunden. Dies bedeutete eine massive Einschränkung des wissenschaftlichen Betriebs.

Innerhalb von wenigen Wochen ist es dem SCC gelungen, eine 2-Faktor-Authentifizierung (2FA) für alle HPC-Systeme mit zeitbasierten Einmalpasswörtern (TOTP) einzuführen. In Kombination mit der 2FA ist auch die Nutzung von SSH-Keys wieder möglich. Sowohl die 2FA-Tokens als auch die SSH-Keys werden zentral über bwIDM verwaltet. Bei den SSH-Keys erfolgt eine Unterscheidung zwischen Schlüsseln für interaktive Nutzung und solchen für die Automatisierung von Workflows (sog. kommandobezogene Keys). Weitere Betreiber aus dem bwHPC-Verbund planen die Einführung der 2-Faktor-Authentifizierung auf Basis der für das bwIDM neu entwickelten Komponenten.

Detaillierte Informationen zu den neuen Abläufen und Regeln finden sich unter anderem in der Nutzerdokumentation des bwUniCluster 2.0.

bwSFS – Storage for Science

bwSFS – Storage for Science

The Universities of Tübingen and Freiburg have teamed up to build a federated storage system for data intensive computing and research data management: bwSFS (“Storage for Science“). It has been co-funded by the German Research Foundation (DFG), the Ministry of Science, Research and the Arts Baden-Württemberg (MWK), the Universities of Tübingen and Freiburg and individual research groups. The principal design of the systems aims for more functionality than just a vast but simple data sink. Therefore, in addition to several Petabytes of newly available storage for scientific research data, there will be additional state-of-the-art components to facilitate research data management tasks for its users.

The system is set up at several locations in Tübingen and Freiburg to provide redundancy and fail-safe operation. To allow fast data access to bwSFS at the universities of Konstanz and Stuttgart, cache-servers are placed at these universities. bwSFS will be jointly operated by the “Zentrum für Datenverarbeitung (ZDV)“ in Tübingen and the Computing Center in Freiburg. Scientific guidance is discussed within the Research Data Management Group (RDMG), a community that has been initially formed in the wake of the procurement of the hardware and software solutions.

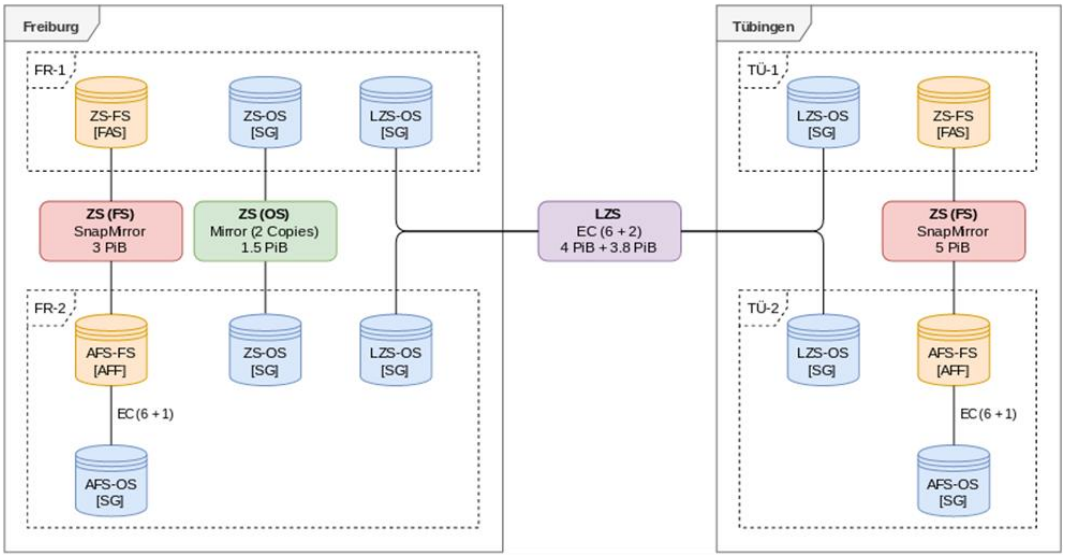

Figure 1 --Schematic layout of the Storage-for-Science (bwSFS) system (ZS - Zentralspeicher, LZS - Langzeitspeicher, AFS - Ausfallspeicher, FS - Filesystem, OS - Objektspeicher). The cache servers residing in Tübingen, Freiburg, Konstanz and Stuttgart are not shown.

bwSFS – Storage for Science

Installation and basic configuration of the bwSFS system is currently nearing completion. Initially, there will be standard services provided, such as file shares (NFS and Samba) and object storage (S3). The technical foundation for the operation of the storage and research data management resources will be based on InvenioRDM. It will be under construction for a while, since this is not a turn-key solution, but rather an ongoing endeavor.

In the long run, bwSFS will provide support for the active handling of research data and its annotation at all four participating universities. A significant share of the data volume is reserved for the scientific communities that participated in the application. This includes the HPC communities in Tübingen (BioInformatics, Astrophysics) and Freiburg (Elementary Particle Physics, Neuroscience, Microsystem Engineering and Material Sciences) as well as the Bioinformatics community represented by the de.NBI project. In this regard, bwSFS will be a backbone infrastructure for the SDC BioDATEN, the NFDI GHGA and the NFDI DataPLANT.

Planned higher level services to be offered beyond file shares and object storage include GitLab repositories for versioning of data and code, the InvenioRDM system for data publication and community supported services like the OMERO database for imaging data among others. Their implementation will take place gradually in the coming months. Based on the current state of planning, we assume full availability from Q2/2021.

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bwsfs-support@rz.uni-freiburg.de

contact Tübingen:

bwsfs@zdv.uni-tuebingen.de

Written by Bernd Wiebelt, Dirk von Suchodoletz, Kolja Glogowski and Mark Seifert/University Freiburg;
Ulrich Hahn and Jens Krüger/University Tübingen

Current bwHPC Course Offers & Online Vampir Workshop

Level	Topic	Title	Begin	End	Location
Advanced course	Programming	Fortran for Scientific Computing	07.12. 2020	11.12. 2020	Online hlrs.de/training/2020-12-07-ftn2
Basic course	Parallel programming	Matlab on HPC	10.12. 2020	10.12. 2020	Online https://training.bwhpc.de
Advanced course	Programming	Modern C++ Software Design	02.03. 2020	05.03. 2020	Online hlrs.de/training/2021-03-02-cpp1
Advanced course	Programming	Modern C++ Software Design	04.05. 2020	07.05. 2020	Online hlrs.de/training/2021-05-04-cpp2

Ein Workshop zur "Performance-Analyse mit Vampir und Score-P"
findet am 18. März 2021 von 13 – 17 Uhr statt. Der Workshop erfolgt Online mit WebEx.
Experten der TU Dresden erklären Tracing mit MPI, OpenMP, OpenCL und CUDA-parallelen Anwendungen auf den bwHPC-Systemen. Link zu Webex:

https://hs-esslingen.webex.com/hs-esslingen/j.php?MTID=m0c687f9c44f9bb0852e3e6042ef9b00b

TECHNISCHE UNIVERSITÄT DRESDEN

On March 18th, 2021, experts of TU Dresden will meet in a virtual workshop using WebEx. They will explain tracing and performance analysis using MPI, OpenMP, OpenCL and CUDA parallel applications on the bwHPC systems. The workshop will be held in German.

Written by Rainer Keller/University of Applied Science Esslingen

E-Science-Tage 2021

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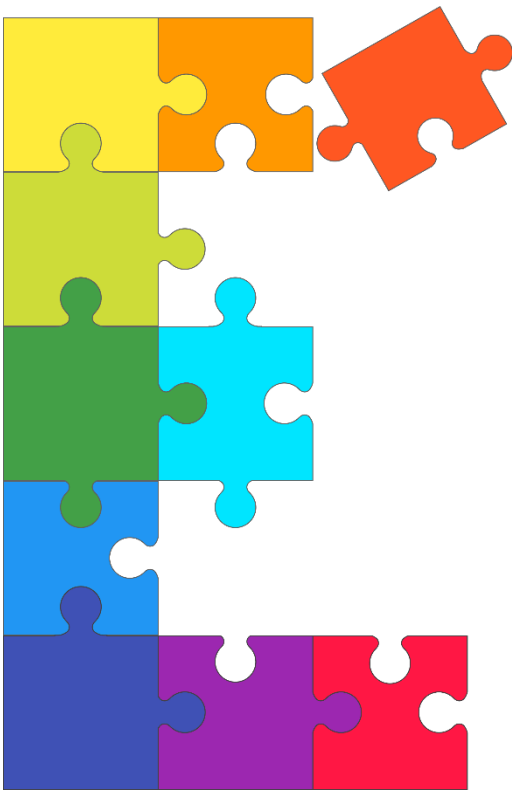
E-Science-Tage 2021: Share Your Research Data

Vom 4. bis 6. März 2021 finden die E-Science-Tage 2021 "Share Your Research Data" als Online-Konferenz statt.



Durch den Austausch von Forschungsdaten können Wissenschaftlerinnen und Wissenschaftler von der Möglichkeit profitieren, vorhandene Datensätze wiederzuverwenden und dadurch die Effizienz des gesamten wissenschaftlichen Fortschritts steigern.
Der Datenaustausch erzeugt mehr Transparenz und kann als qualitätssichernde Maßnahme betrachtet werden. Er begünstigt neue Kollaborationen, fördert die interdisziplinäre und internationale Zusammenarbeit und steigert letztlich den Erkenntnisgewinn. All diese Aspekte dienen der guten wissenschaftlichen Praxis und sichern den hohen Qualitätsstandard unserer Forschung.

Wir freuen uns, mit den E-Science-Tagen 2021 eine Plattform zu bieten, die diesen wichtigen Forschungsaspekt in den Mittelpunkt rückt.

Der CALL FOR CONTRIBUTIONS für die E-Science-Tage 2021 ist eröffnet!
Abstracts können bis 18.12.2020 eingereicht werden.
Link zu den E-Science-Tagen 2021
Folgen Sie uns auf Twitter.

Organisations -Team der E-Science-Tage 2021
e-science-tage@uni-heidelberg.de

E-Science-Tage 2021

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Die E-Science-Tage 2021 widmen sich unter anderem folgenden Fragen:

- ✓ Wie hoch sind der Nutzen und das Risiko für den Austausch vorhandener Forschungsdaten?
- ✓ Wie kann der Datenaustausch dazu beitragen, mehr Transparenz zu erreichen?
- ✓ Wie trägt der Datenaustausch zur Verbesserung der Forschungsqualität und zum wissenschaftlichen Fortschritt bei?
- ✓ Wie können digitale Infrastrukturen den Austausch von Forschungsdaten erleichtern?

E-SCIENCE-TAGE

E-Science-Tage 2021: Share Your Research Data
March 4 - 6, 2021- Online conference

By sharing research data, scientists benefit from reusing existing data sets in order to increase the efficiency of scientific progress. Data exchange creates more transparency and can be viewed as a quality assurance measure.
In addition sharing research data brings new collaborations, which can promote gaining knowledge. All these aspects will serve good research practice and ensure the high quality standard in research.

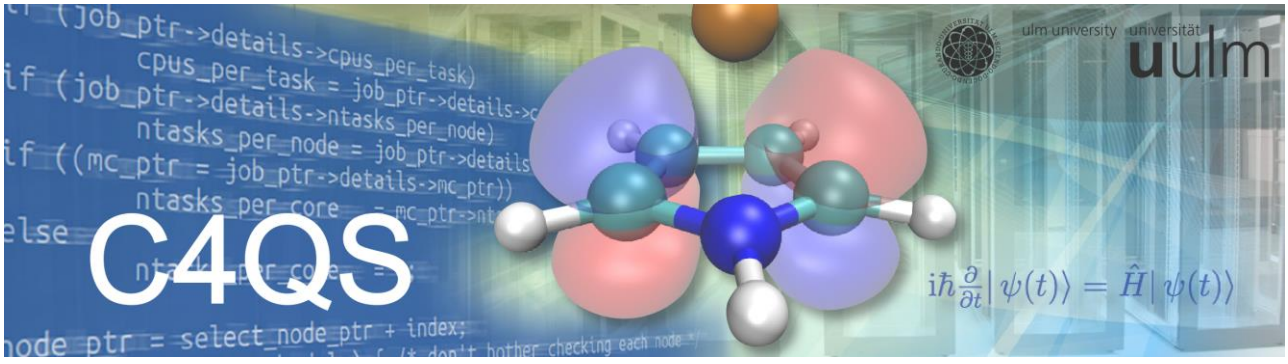
Written by Nina Mohammadianbisheh/Heidelberg University

We present our Competence Center

Introducing the bwHPC Competence Center for Computational Chemistry and Quantum Sciences

The Competence Center for Computational Chemistry and Quantum Sciences (C4QS) is the stage where scientific expertise and computer system knowledge coexist for the benefit of all researchers. It serves as a contact point for researchers seeking guidance for the best use of the bwForCluster JUSTUS 2 to solve their scientific problems by means of computational methods.

The competence center also tries to actively identify inefficient use of compute resources and offers help in these cases as to maximize the efficiency and available resources for all users. The members of the C4QS team are hardware, software and science experts located at several universities in Baden-Württemberg. They provide services for all scientists in the field of Computational Chemistry and Quantum Sciences across the state of Baden-Württemberg. C4QS is one of seven competence centers in Baden-Württemberg under the umbrella of the bwHPC project and funded by the Ministry for Science, Research and Art of Baden-Württemberg.



We present our Competence Center

Founded in 2014 as Competence Center for Computational Chemistry, the scientific focus has been expanded in 2019 to cover Condensed Matter Physics, Quantum Optics and other Quantum Science related research subjects as well. Research groups from these additional topics did support our JUSTUS 2 grand application and are meanwhile frequent users of the cluster. Extending the scope of the competence center is quite challenging since additional knowledge and new techniques have to be established beyond the classic approaches in this computational community. For example machine learning, GPU acceleration, FPGAs and data intensive computing are new technologies which are currently made available on the cluster. Some of these technologies open new research fields or allow a deeper insight into existing ones. The GPUs for example speed up certain calculations like molecular dynamics by a considerable factor and thus allow to tackle much larger systems or simulate processes on longer time scales. Still, using GPUs efficiently is not common to most chemistry software and scientists as well as software developers are just gaining experience using these new tools.

Up to now C4QS has supported more than 600 scientists in 150 research projects who published more than 550 scientific papers, to which results obtained on the bwForCluster JUSTUS have contributed. All kinds of computational chemistry and, recently, quantum science related research topics are covered. Besides the efforts to help with technical or scientific problems, the competence center also offers more extensive cooperation with some research character by so called "Tiger Teams". This cooperation covers both, technical and research aspects, to allow a deeper dive into more challenging questions.

You can reach the bwHPC Competence Centers either via the support portal https://www.bwhpc.de/supportportal by assigning your ticket to the corresponding support unit or you can contact the competence centers by email: https://www.bwhpc.de/teams.php

Written by Christian Mosch, Frank Wagner, Jan Kucera, Jürgen Salk and Karsten Siegmund/Ulm University;
Rainer Keller/University of Applied Science Esslingen

Winter greetings

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"To appreciate the beauty of a snowflake it is necessary to stand out in the cold."

Aristotle

The bwHPC team wishes you a nice and healthy winter time.

Imprint

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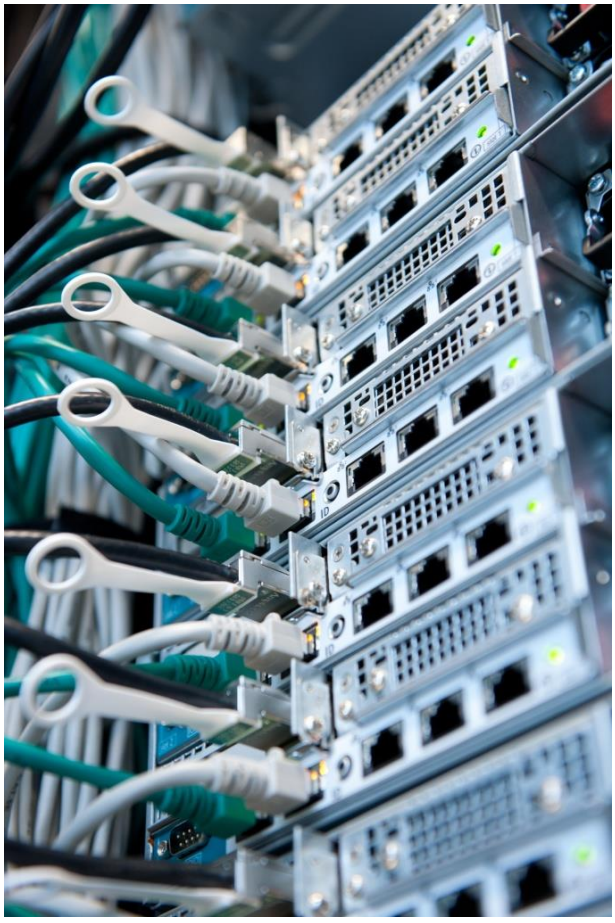

Photo by Elvira Eberhardt/Ulm University

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