

Newsletter 04/2023

Welcome to the newsletter of the dtec.bw project hpc.bw. If you want to subscribe to the newsletter, please send a message with subject line "Subscription hpc.bw Newsletter" to info-hpc-bw@hsu-hh.de.

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Seminar Series Computation & Data in WT24

In the winter trimester (WT 2024), we warmly invite you to the upcoming talks in our seminar series Computation & Data at the HSU and look forward to exciting discussions on the topic! In addition to attending in presence at the HSU, it is also possible to participate digitally via MS Teams.

Date	Room	Speaker	Title of lecture
31.01.2024; 16:00-18:00	Mensa Room 0001	Lukas Augustin (HSU)	SmartShip: AI-Driven Maritime Rescue - Enhanced Readiness and Detection in Search Operations
		Volker Gravemeier (AdCo Engineering ^{GW} GmbH)	A Novel Multiphysics Computational Method for Coupled Simulations of Tribological Systems
28.02.2024; 16:00-18:00	Mensa Room 0001	Ali Khalifa (HSU)	Neural Network-Based Multiscale Modeling of Deagglomeration due to Wall Impact and Collisions
		Denis Kramer (HSU)	t.b.a.
27.03.2024; 16:00-18:00	Mensa Room 0001	Sebastian Brandstätter (UniBw M)	Sensitivity Analysis for Biomechanical Models
		Ruben Horn (HSU)	Energy Efficiency of Molecular(-Continuum) Simulations

To subscribe to the seminar mailing list, send an e-mail to info-hpc-bw@hsu-hh.de, subject line „Subscription Seminar Computation & Data“. For more information, [click here](#).

3rd Call for Projects for Performance Engineering

In the context of the 3rd Call for Projects for Performance Engineering, we invite all research groups of the Universities of the Armed Forces Hamburg and Munich to submit proposals on project outlines for performance engineering. Projects for performance engineering are meant to enable computer-aided research, implementations and software parallelization, as well as the assessment of discipline-specific questions with the help of fast algorithms. Within the project framework, support for respective performance engineering tasks will be provided by research assistants as part of the hpc.bw project funding.

The period for carrying out the projects is from 01.04.2024-31.12.2024. Proposals are submitted by filling out the application form until 16.02.2024 and sending it via e-mail to info-hpc-bw@hsu-hh.de.

We are looking forward to receiving your projects ideas until 16.02.2024!



You can find more information on our website [here](#).

To read the call text, click [here](#), and to check the application form, [here](#).

Anniversary: One Year CBRZ and HSUPER

Congratulations to our HSUPER machine and the container-based HPC center (CBRZ), which have officially only turned “1” this December!

This is a good time to look into statistics from this first year of CBRZ/HSUPER.

The Users: The number of users grew from 60 from last December (who already gained access for early system testing over the prior four months) to 153. This includes collaborators, particularly from UniBw M, but also from other (dtec.bw-related) partner institutions.

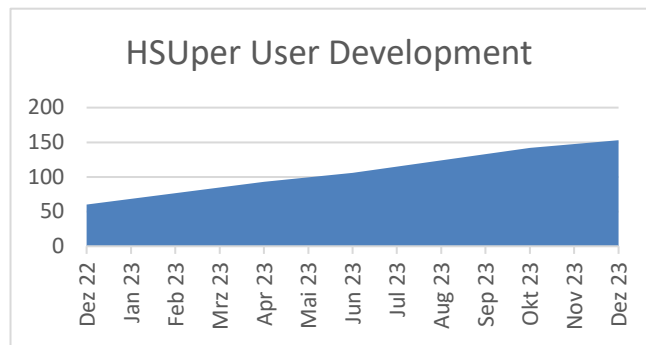


Figure 1: HSUPER user development over the last year

The Jobs: While HSUPER was only used to ca. 23% in December 2022, cluster utilization times have in the meanwhile accumulated to ca. 65% of the entire available HSUPER compute time in the second week of December 2023, with several high-utilization hot spots, cf. Figure 2. Also, the percentage of successfully completed jobs grew from 63% in the first 5 months to 92% during summer 2023 (June to October), demonstrating that users adapted well to the new system.

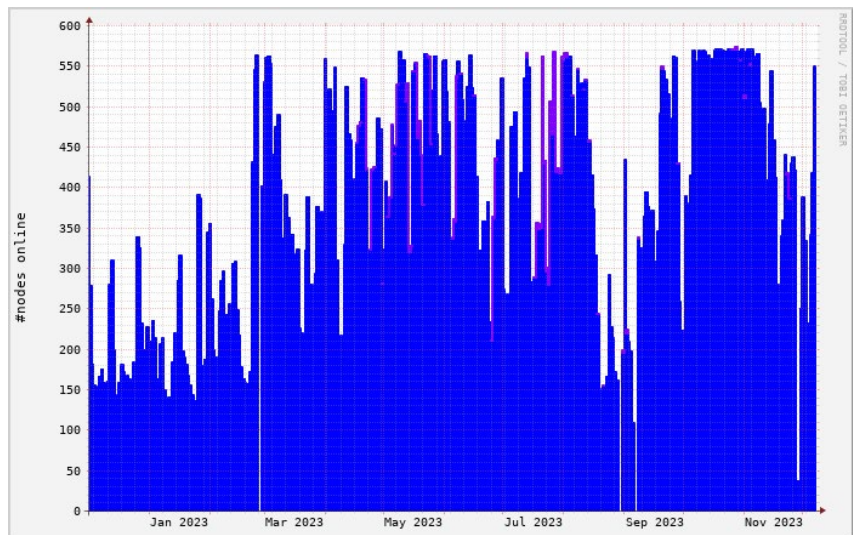


Figure 2: Number of compute nodes that were online over the last year. Offline phases of nodes are typically due to automated shutdowns to save energy.

The System: Several updates to our software stack have already been necessary in this first year and have been successfully installed. In particular, we had few issues with our BeeGFS file system throughout the year (e.g., reduced performance), which could, however, all be addressed and resolved. Also, our GPU nodes have been upgraded over the year to comprise node-local scratch space of 894 GB.

HSUper User Meeting

The next HSUper user meeting will be held on Friday, 9 February 2024 at 14:00 in seminar room 0108 in building H1. The user meeting is open to every HSUper user to share experiences. Feel free to join us. Please send an e-mail to info-cbrz@hsu-hh.de in case of any questions regarding the meeting.

Insights into the Questionnaire-based Survey of the First HSUper Workshop on 28.09.2023

In the scope of our recent HSUper workshop on 28.09.2023, we conducted a questionnaire-based survey to further shape our competence platform offers (workshops, online material, etc.) in the future. We received a total of 28 completed questionnaires.



Scientific disciplines

In the Figure 3, you can see the distribution of scientific disciplines among the 28 participants who completed the questionnaire. This reveals a broad range of scientific disciplines, each with a different focus, in which the workshop participants work.

These include, for example Engineering with focus on Structural Optimization or Geodesy, Data Science such as Statistics as well as Computer Science with regard to Cloud Computing and Neural Networks. Moreover, there were also participants from the Social Science such as Political Science, Economics with focus on Operational Research as well as Natural Science with focus on Cognitive Neuroscience.

Figure 3: Distribution of scientific disciplines, N = 28

Needs and requirements

The fact that the HSUper workshop addressed a heterogeneous target group was also evident in the evaluation of the questions about needs and requirements. In the course of this, we asked, what were the seminar topics that caught the greatest interest. Figure 4 shows clearly that the participants are as diverse as the needs that led to their participation in the workshop. The majority was interested in how to use module systems, how to allocate nodes of HSUper interactively or how to write scripts as well as to utilize the parallel storage system.

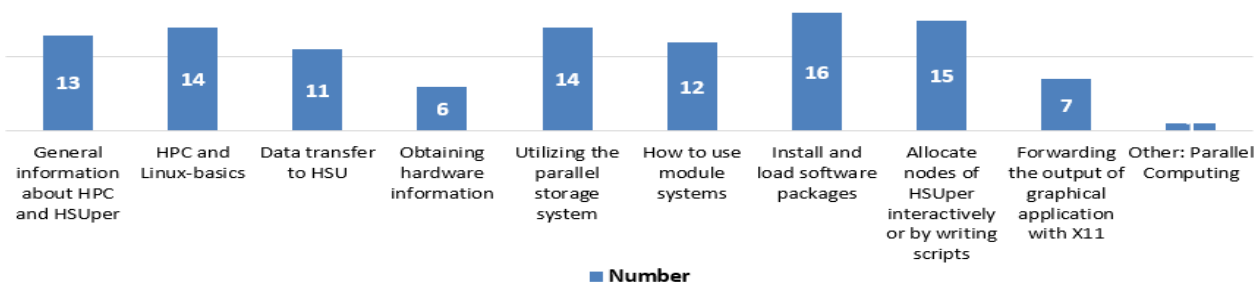


Figure 4: „Which seminar topic caught your greatest interest?“ (multiple answers possible); N = 28

In preparation for potential further offerings of hpc.bw, we also asked the participants for additional interest in topics related to HPC or supercomputing. Therefore, we categorized topics close to what we offered in the first workshop setup and also gave the opportunity to give individual answers. The heterogeneous responses, which can be seen in Figure 5, can be clustered into the following three thematic blocks: (a) Performance

Engineering, Software Development and Code Optimization, (b) HPC Knowledge/Fundamentals and Environments, (c) Big Data Analysis.

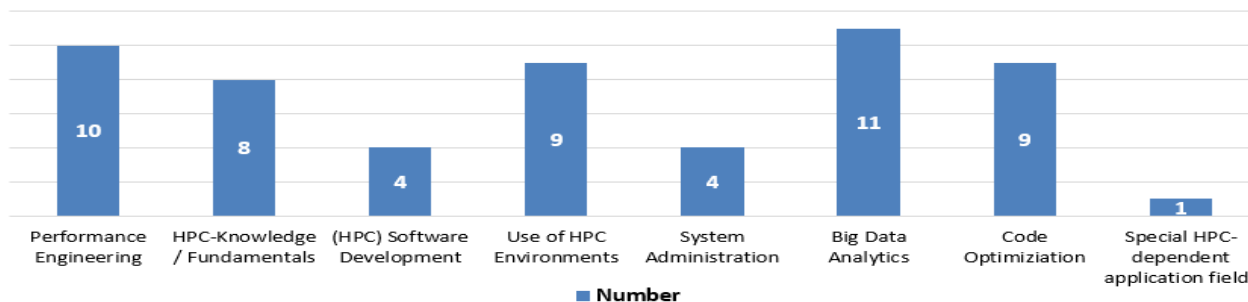


Figure 5: "In which of the following topics are you especially interested?" (multiple answers possible); N = 28

Outlook

Based on the feedback obtained through the survey, we will provide a second workshop on 18/19 April 2024, see below. This time the workshop is split into two days to better address both beginners and advanced users separately and to have more time for each group. We also plan some space for networking between both groups.

Announcement: Second HSUPER Workshop for Beginners on 18.04.2024 and for Advanced Users on 19.04.2024

We cordially invite you to the HSUPER workshop for beginners on 18.04.2024 and for the HSUPER workshop for advanced users on 19.04.2024 to gain a comprehensive insight into HPC and an introduction to using the supercomputer HSUPER!

You are welcome to attend the workshops and to learn along theoretical insights as well as practical examples more about the broad word of HPC. The workshop will take place on-site at the HSU.

The HSUPER workshop for beginners focuses on the one hand on topics such as an introduction to HPC, Linux basics, and data transfer to HSUPER as well as obtaining hardware information. On the other hand, you will learn how to use the module system to load installed software, the interactive compute node allocations, and write and submit Slurm jobs.

The second HSUPER workshop for advanced HPC users is organized around four thematic blocks: Firstly, HPC-competencies, and secondly, HPC Knowledge and Environments. Moreover, big data analysis as well as best practices for HPC software and projects will be a part of the HSUPER workshop for advanced users.

[Here](#) you can find more information on our website.

Have a look into the schedule for the HSUPER workshop for beginners [here](#):



And [here](#) for the advanced users:

Call for Posters: HSUPER Workshop for Beginners and Advanced Users

We also invite you to present a poster at both HSUPER workshops. The aim is to illustrate the variety of topics and methodological approaches in the wide discipline of HPC, to highlight different research perspectives as well as to enable an interdisciplinary exchange, all at a low-effort level.

[Here](#) you can find more information about the Call for Posters:



Please register for the workshop until 16.02.2024 by sending an e-mail with subject line "Registration: HSUPER workshop beginner" or "Registration: HSUPER workshop advanced user" to workshops-hpc.bw@hsu-hh.de. Please inform us during registration if you plan to bring a poster.

Project Update: benEFIT

We concluded our work on the project ‘benEFIT- Numerical simulation of non-destructive testing in concrete’. This project aimed to optimize a Fortran program which simulates sound waves in inhomogeneous concrete and is used by the professorship for engineering materials and building preservation (HSU) to enhance the accuracy of non-destructive testing methods of concrete.

Initial changes to the program included the application of fitting MPI types as well as the introduction of some best practices in coding. Further performance-relevant changes reduced division operations, merged some memory intensive loops (loop fusion), and collapsed some artificial inflated spatial information, resulting in an overall runtime reduction of more than 50%. The collapse and fusion improved the operations per memory load (operational intensity) and represented the major changes for these performance gains.

A large part of our work involved the incorporation of the I/O libraries NetCDF and TIXI. TIXI is used to enable the configuration of benEFIT via XML files. NetCDF enables restarting/checkpointing simulations and the writing of portable simulation results. This reduces the file sizes of the simulation results and facilitates the processing with additional tools.

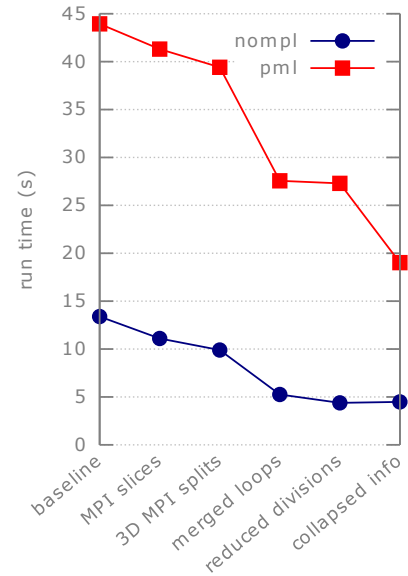


Figure 6: Changes of the program run times over the applied major changes. Displayed for two covered test cases.

Project Update: Logistics and Optimization

In hpc.bw, one sub-project is dedicated to investigating how available mixed-integer mathematical optimization solvers are already able to exploit parallel computing power of the shelf.

In the plots, a runtime comparison of the software Gurobi with various threads numbers for the benchmarks ta061, ..., ta069 (time-dependent traveling salesman problems) is shown.

Each benchmark has a different color (see legend). Each marker in the plots corresponds to 1 run of a computation on the respective hardware systems (HSUper/Intel Xeon Platinum 8360Y, AMD EPYC 7763, ARM FX700), whereas the numbers in 1, 2, ..., 128 represent the number of threads used. However, no results are included in the comparisons with ARM for the setups ta062 with 1 thread as well as ta066 with 2, 4 or 32 threads since these setups failed on this system.

The plots illustrate that the AMD and HSUper systems are expectedly faster than ARM, whereas there is no clear winner between HSUper and AMD. In a next step, we want to study the influence of performance variability as well as the hardware characteristics that favor HSUper and AMD. Are the performance differences only based on the clock speed? And also, how about energy consumption, comparing ARM with the other systems?

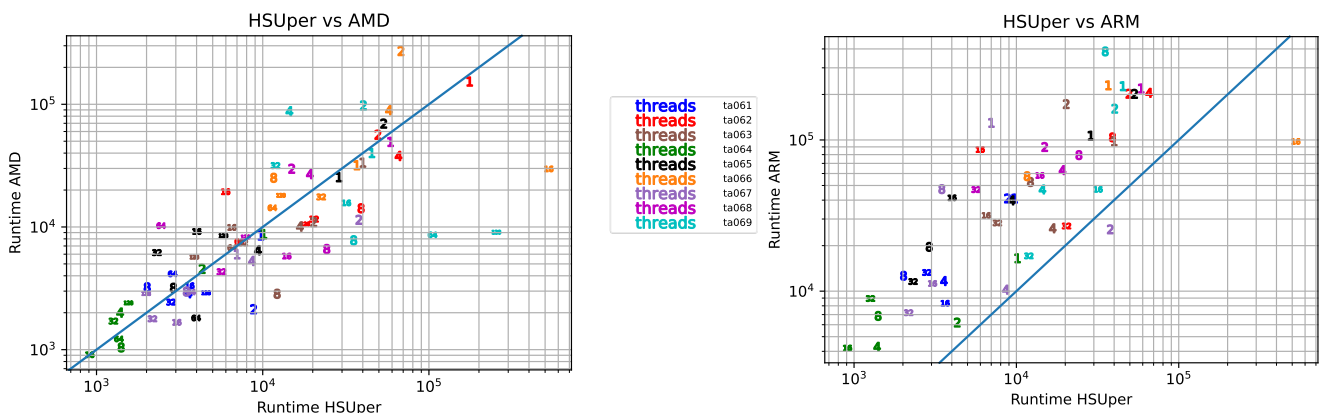


Figure 7: Performance of time-dependent traveling salesman problem solving on three hardware architectures

Closing Words for 2023



©David Ernst, Alexander Kolling, Marie Rathmann, Yannis Schumann, Henrik Weitzel

An exciting year comes to an end: our supercomputer HSUper is now already for one year on the campus of HSU, the interactive scientific computing cloud has just been installed this summer, further successful optimizations have been achieved as a part of our performance engineering projects and the next call has been published, many exciting interdisciplinary lectures in our seminar series “Computation & Data” have been used to disseminate the digital, scientific HSU and Unibw M landscape, a workshop for HSUper users was organized and several conferences were attended to strengthen HPC knowledge, transfer and research – just to name a few facts. 😊

Traditionally, December is the time in which children can’t wait for Santa Clause (or the Christ Child – collaborative efforts have very old roots 😊) to bring some presents for them. Admittedly, this spirit feels a bit to carry over to HPC and dtec.bw these days, with all researchers awaiting the decisions on dtec.bw continuation in the new year. Of course, we strive to increase the “Santa probability” and conduct research, we support each other in interdisciplinary collaborations, we educate, train and support.

By “we”, it is not only the hpc.bw team that I have in mind here, but also the 153 HSUper users! I want to thank all of you for your contributions throughout the last year. Also, a big thank you goes out to our collaborators at Opheo Solutions, algorithmica technologies and our CBRZ/HSUper vendor MEGWARE. I am very much looking forward to what the new year will bring and keep fingers crossed for '25-'26. 😊

Merry Christmas and a happy new year 2024,

Philipp Neumann

