

Newsletter 04/2024

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.

Contents

Seminar Series Computation & Data in WT25	1
4 th Call for Projects for Performance Engineering	2
Anniversary: 2nd Birthday of HSUper.....	2
HPC Portal: Digital Workshops	3
Project Update: Density Functional Theory Calculations of Positron Lifetimes.....	4
Project Update: Nozzle Design in Cold Spray Applications	4
(Project) Update: Logistics and Optimization.....	4
Project Update: Job Scheduling Algorithm Implementation.....	5
Closing Words for 2024	5

Seminar Series Computation & Data in WT25

We warmly invite you to the upcoming talks in our seminar series *Computation & Data* at the HSU in the winter trimester (WT25) 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
29.01.2025 16:00-18:00	seminar room 403	Natalie Rauter (HSU)	How to predict material behavior by utilizing neural networks
		Jasper Ibnamar (Laboratoire d'informatique, parallélisme, réseaux, algorithmes, distribués)	Performance profiling on modern HPC computer systems: techniques and tools
26.02.2025 16:00-18:00	seminar room 403	Gerhard Schreiber (HSU)	Data Toxicity: Observations and Reflections from a Techno-Ethical Perspective
		Kathrin Welker (HSU)	Constrained shape optimization in shape spaces: Models raising from deterministic to stochastic settings
26.03.2025; 16:00-18:00	seminar room 403	Markus Klein (HSU)	Towards LES of Liquid Jet Atomization Using an Eulerian-Lagrangian Multiscale Approach
		Marcel Dickmann (HSU)	Two-Component Density Functional Theory Calculations of Positron Lifetimes at HSUper

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](#).

4th Call for Projects for Performance Engineering

In response to the 4th Call for Projects for Performance Engineering, we invite research groups affiliated with the Universities of the Armed Forces in Hamburg (HSU/UniBw H) and Munich (UniBw M) to submit proposals outlining projects that align with the objectives of performance engineering. The primary aim is to facilitate computer-aided research as well as investigate discipline-specific questions through the application of efficient algorithms, code optimization and parallelization. Within the project framework, researchers will have access to support from research assistants, courtesy of the hpc.bw project funding, to join forces on performance engineering tasks.

The period for implementation of the projects is from 01.04.2025-01.04.2026. To participate, please submit your proposals by completing the application form no later than 14.02.2025 via email to info-hpc-bw@hsu-hh.de. We are looking forward to receiving your project ideas!

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

You can find more information on our website [here](#) or scan the QR Code:



Anniversary: 2nd Birthday of HSUPER

Congratulations to HSUPER and the container-based HPC center (CBRZ) which have been in operation officially for two years now!

This is a good time to review the year and look into some statistics. The number of users grew from 153 up to 198 during the past 12 months. The average utilization has also increased over time. While HSUPER was only used to 23% initially in December 2022, cluster utilization was mostly above 90% in the past weeks in 2024, see Figure 1. Two maintenance downtimes can be seen clearly in the figure, where the cooling towers were moved down from the container building and moved back on top of the newly constructed roof. These maintenance times have also been used to modernize and update our software stacks, including the packages available in the module system, compilers and the OS software stack.

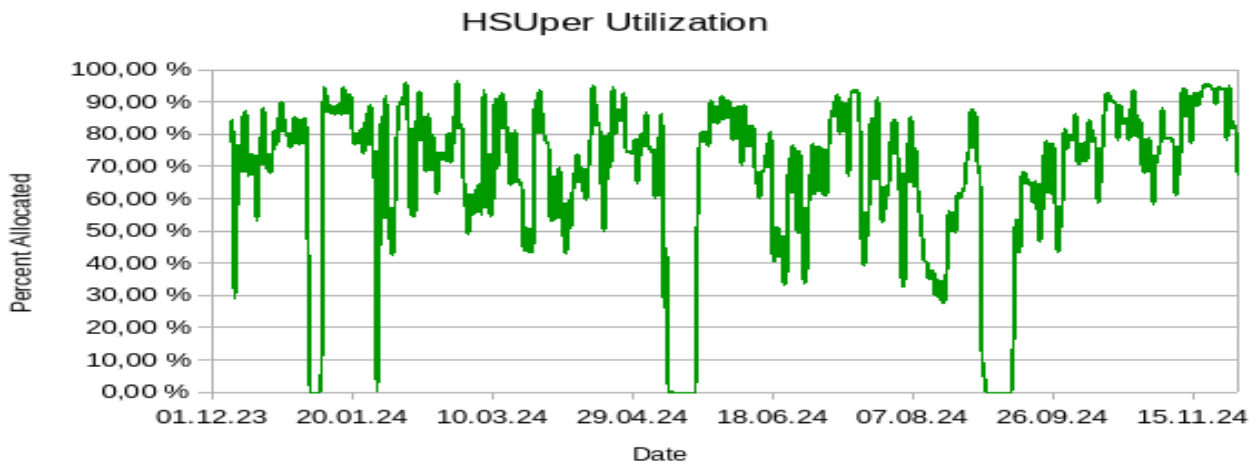


Figure 1

HPC Portal: Digital Workshops

We are pleased to announce that three new workshops have been added to the HPC Portal. As part of the revitalized HSUPER Workshops series, originally developed as an on-site training comprising six modules, these digital trainings now offer a flexible and self-paced learning experience. Specifically designed for HSUPER users, they provide a means by which individuals can independently acquire the necessary competencies to effectively utilize HPC resources.

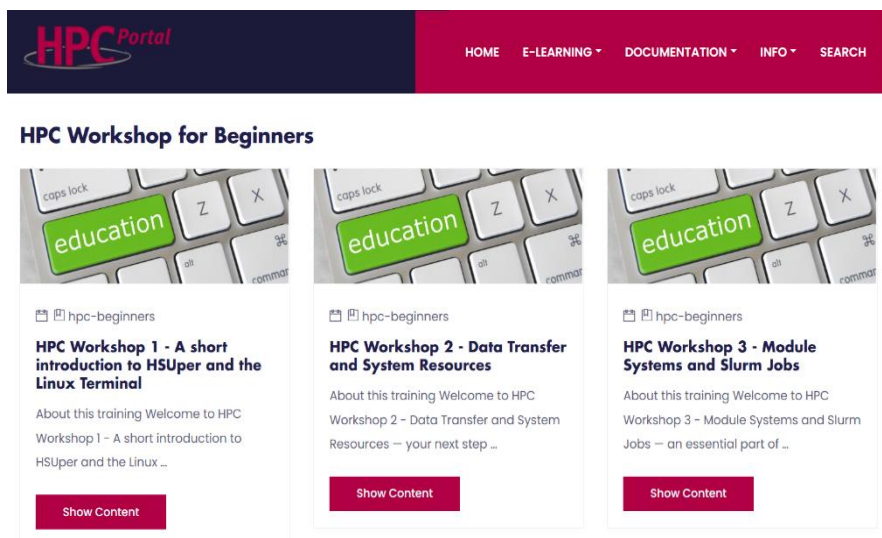


Figure 2

[Workshop 1 - A Short Introduction to HSUPER and the Linux Terminal](#)

This workshop is perfect for those starting out with HSUPER and the Linux terminal. The training begins by introducing the prerequisites for accessing the HPC infrastructure at HSU and familiarizing participants with the HSUPER system. Through a guided exploration of the Command Line Interface (CLI), attendees will develop an understanding of how to navigate and interact with the system.

Subsequently, the workshop focuses on managing text files, encompassing viewing, creating, and deleting them. A practical exercise is integrated into the training, enabling participants to apply their new skills in a real-world context and enhance their problem-solving abilities.

The training then proceeds to cover the organization of directories, including creating, deleting, and modifying them. Finally, it provides an introduction to scripting and working with environment variables, laying the foundation for further learning and exploration within the HSUPER system.

[Workshop 2 - Data Transfer and System Resources](#)

This training empowers participants to effectively transfer data to and from HSUPER by imparting essential skills in this area. The course of instruction begins by providing a comprehensive overview of the necessary information required for task management, encompassing an understanding of storage system details, hardware specifications, nodes, and partitions.

The concluding segment of the workshop provides critical insights into current cluster utilization, enabling participants to optimize their workload management strategies and plan resource requirements more effectively in anticipation of future needs.

[Workshop 3 - Module Systems and Slurm Jobs](#)

Targeted at users seeking to develop proficiency in software module management and job scheduling, this workshop provides a comprehensive introduction to these essential skills. The training commences with an exposition on module systems, where participants will acquire knowledge on how to enumerate, load, and unload software modules.

The subsequent section of the workshop focuses on interactive allocation of compute nodes, allowing participants to engage in hands-on exercises that consolidate their understanding of these critical tasks. Finally, attention turns to Slurm job management, wherein participants will learn how to craft, configure, and submit Slurm jobs, as well as manage the job queue by updating queued jobs and cancelling running jobs.

Through this training, participants will acquire a thorough grasp of software module management and job scheduling, thereby empowering them to optimize their HPC workflows.

Project Update: Density Functional Theory Calculations of Positron Lifetimes

This project aimed to support the Institute of Applied Physics and Measurement Technology at UniBw Munich in setting up a simulation workflow needed for their research using Positron Annihilation Lifetime Spectroscopy. The institute's research is accompanied by Component Density Functional Theory calculations carried out via the open-source software ABINIT.

We provided assistance in setting up ABINIT 8 and 9 on our cluster, and tested the software with provided test cases to find ideal operation parameters. We communicated our findings and the manual installation steps for ABINIT 9 as well as the installation steps using Spack for ABINIT 8.

Project Update: Nozzle Design in Cold Spray Applications

The project aimed to support our project partner in his transition from ANSYS-Fluent workflow on smaller work-stations to the usage on a cluster with more resources. This was necessary in order to process more computationally intensive models and setups.

We provided a dedicated virtual machine via our ISCC computing platform, allowing for interactive ANSYS GUI interaction during the transition to a purely job submission-based approach. We also provided instructions on how to parallelize ANSYS-Fluent calculations on HSUper, as well as general guidance on scripting ANSYS workbench interactions to manage non-interactive workbench computations using Slurm.

(Project) Update: Logistics and Optimization

One of the hpc.bw subprojects, namely “Logistics and Optimization”, is dedicated to the investigation of mixed-integer mathematical optimization solvers available in the market, and how they can exploit parallel computing power off the shelf. In the plot, a comparison of the CPU power usage in watt [W] for the software Gurobi with default parameters (i.e., the number of threads is determined automatically with a soft limit of 32) for the time-dependent travelling salesman problems ta061, ..., ta069 is shown. The table shows the corresponding runtimes in hours and minutes [HH:MM], CPU power in kilowatt-hour [kWh] and the maximal RAM usage in gigabyte [GB]. For the experiment, one fat memory node of HSUper (2x Intel Xeon Platinum 8360Y, 1 TB RAM) is always used exclusively. “Split in 9 parts” means that we split the node in 9 parts with each part using 8 cores to solve one of the problems, “simultaneous” means that we start all 9 Gurobi runs simultaneously and let the operating system determine how the up to $9 * 32 = 288$ Gurobi threads are distributed over the 72 available cores, and “sequential” means that one Gurobi run starts after another run finished. This indicates that solving several problems simultaneously increases the RAM usage as well as the runtime of each individual run. However, the wall clock time as well as the CPU power used to solve several models decreases significantly by running several models simultaneously.

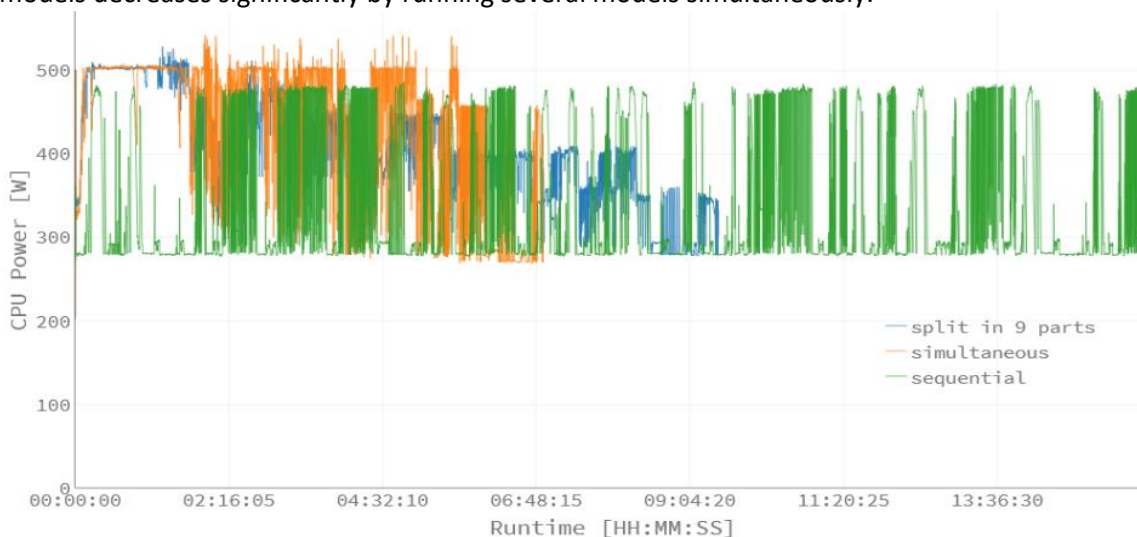


Figure 3

	Split in 9 parts	Simultaneous	Sequential
Runtime [HH:MM]	9:30	6:55	15:53
CPU Power [kWh]	3.90	3.02	5.47
Max RAM usage [GB]	292	293	51

Table 1

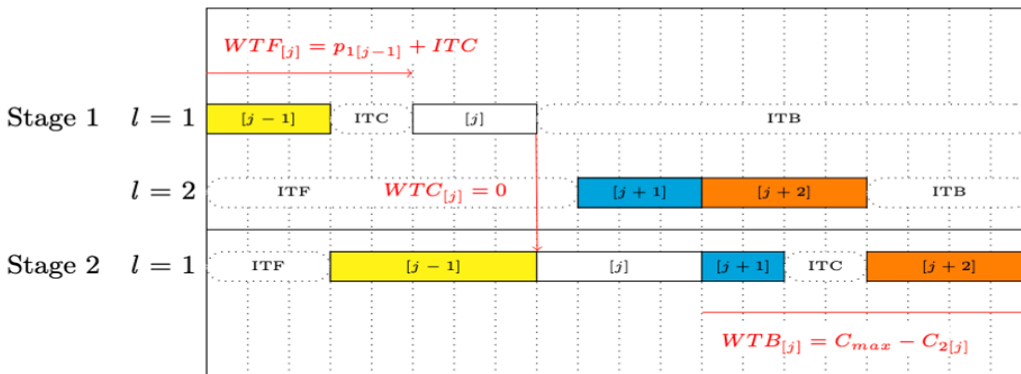
Project Update: Job Scheduling Algorithm Implementation

This project supports the Institute for Business Administration, Management Science and Operations Research at HSU, in developing an efficient algorithm for the two-stages no-wait hybrid flow shop scheduling problem. It is considered as a critical challenge in optimising operations across industries such as manufacturing and logistics. Efficient solutions to this problem help reducing delays, improve resource utilisation, and enhance overall productivity, addressing practical needs in real-world applications.

In the first stage, two machines operate concurrently, while in second stage, one machine executes tasks. Our primary objective is to minimize the total time required to complete all jobs, referred to as the makespan. This goal is achieved through a robust planning and execution framework.

Notably, we have implemented our approach using MATLAB's dynamic programming paradigm, which enables efficient job scheduling. The algorithm adheres to the "no-wait" constraint, wherein tasks are processed continuously without pause or delay between stages.

The implementation exhibits a linear time complexity of $O(n)$, demonstrating an optimal solution for job scheduling in this specific setup. This robust method ensures a strong guarantee for optimizing job scheduling, and a related academic paper is currently being prepared for publication.



WTF = Front waiting time ITF = Front Idle Time
WTC = Core Waiting Time ITC = Core Idle Time
WTB = Back Waiting Time ITB = Back Idle Time

Figure 4

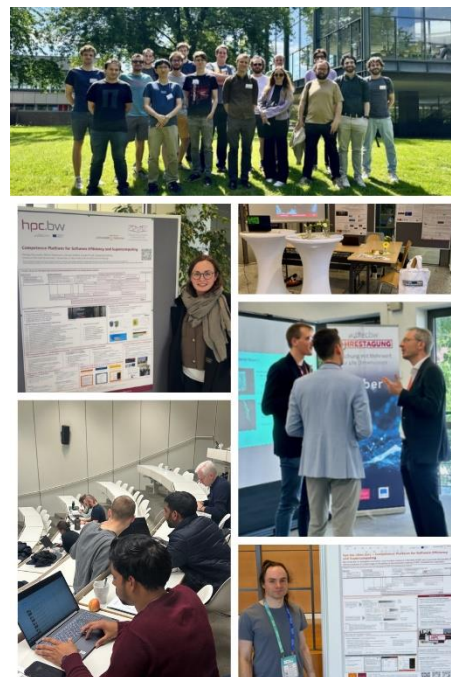
Closing Words for 2024

In the year 2024, many exciting things have emerged in the context of hpc.bw. We achieved several important milestones, such as the approval of a second funding phase (dtec.bw) for the hpc.bw project until December 2026, the implementation of the ISCC cluster with 12 hosts, the publication of the HPC Portal with various learning resources to acquire HPC competences, and Piet Jarmatz as the new head of the HPC Lab.

We also had the opportunity to listen to a total of 20 lectures in our seminar series "Computation & Data" by interdisciplinary researchers who provided us with fascinating insights into current research activities. Furthermore, three HSUper user meetings took place, where not only insights into the utilization of the CBRZ and job scheduling were given, but also an exchange between users was enabled. The hpc.bw project was also present at various events. Starting with the Day of Research on 29.03.2024 at the HSU and just two months later, on 08.06.2024, at the Day of the Armed Forces, also at the HSU. A highlight was, among other things, the poster presentation of the project at the ISC High Performance 2024 in Hamburg and our own information booth in the dimension "Cyber" at the dtec.bw annual meeting at UniBw M from 17.09.-18.09.2024.

As part of the hpc.bw project, the EuroTUG 2024 was organized and took place from 24.06.-26.06.2024 at the HSU, with international researchers joining the event to exchange on the software packages Kokkos and Trilinos.

Not least, we are pleased that we could offer two additional target group-specific HSUper workshops to provide an easy access to HPC computing resources and a competent handling with them. So, an HSUper Workshop for Beginners took place on 18.04.2024 and an HSUper Workshop for Advanced Users took place on 19.04.2024.



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All of these milestones and activities would not have been possible without all the exchange with you – the hpc.bw users, hpc.bw consortium members, dtec.bw team, and many more! Therefore, we would like to express our heartfelt thanks to you! 😊

We are looking forward to the second funding phase with you and are already excited about all the great synergies and activities that will arise from it.



Merry Christmas and a happy new year 2025!