Newsletter 01/2024

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.

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Seminar Series Computation & Data in FT24

We warmly invite you to the upcoming talks in our seminar series Computation & Data at the HSU in the spring trimester (FT24) 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
24.04.2024 16:00-18:00	complex room 1006	Fabian Dethof (HSU)	Simulating “semi-guided” elastic wave propagation in concrete – understanding Impact Echo Data
		Lizzie Neumann (HSU)	Confounder-adjusted Covariances of System Outputs and Applications to Structural Health Monitoring
29.05.2024 16:00-18:00	complex room 1006	Marcus Stiemer (HSU)	Mathematical Optimization and Machine Learning to Support Electronic Design Automation
		Tyron Anton (HSU)	Numerical Calculations using Ansys. Initial Steps and its Challenges
26.06.2024; 16:00-18:00	seminar room 310	Tobias Bohne (UniBw M)	Predicting and Analyzing Violent Conflict using Machine Learning Approaches
		Nils Margenberg (HSU)	Optimal Dirichlet boundary control by Fourier neural operators applied to nonlinear optics

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.

Welcome: New Head of HPC Lab

Starting from 01.03.2024, Piet Jarmatz has taken over the role of the new HPC laboratory manager at HSU.


© Piet Jarmatz

His duties include overseeing daily operations, directing the future development of the CBRZ, supporting system administration and the HPC users, coordinating HPC-aware scientific research and events, and disseminating HPC knowledge. Mr. Jarmatz is excited about the opportunities that HPC offers for science, especially in the context of the rapid emergence of new AI methods for diverse applications. He is eager to start in his new role and is excited to get to know everyone!

Onboarding: Support for New Projects for Performance Engineering

We are very happy to be supporting the following projects from 01.04.2024–31.12.2024 in a variety of ways by research assistants of the hpc.bw team. The aim is to enable computer-aided research, assessment of discipline-specific questions with the help of fast algorithms, implementations, and software parallelization. For optimal support of the projects, the Container-based High Performance Computing Center (CBRZ) HSUper is available.
You can find more information about the individual projects on the website here.

Sebastian Brandstäter (UniBw M)	Enabling global sensitivity analysis of large-scale FEM models using QUEENS
Bahman Daneshian (HSU)	MD-Simulations for damping assessment in MEMS resonators
Marcel Dickmann (UniBw M)	Density Functional Theory Calculations of Positron Lifetimes
Julio Gutierrez (HSU)	Nozzle Design in Cold Spray Applications
Philipp Marienhagen (HSU)	Molecular Monte Carlo simulations on GPUs
Valentina Pessina (UniBw M)	DSMC-based simulation for the development ABEP systems

HPC Portal: Now Available

We are very excited to announce that the HPC Portal is now online! The HPC Portal integrates in the HPC Compentence Platform and its corresponding web presence to enable interested people to learn according to their needs using various learning and training materials. The following offers are currently available: Training in relation to HPC basics, blog posts and newsletters about hpc.bw as well as a HPC glossary with definitions of important HPC related terms. Moreover, there are information about the CBRZ available and instructions on how to access HSUper or ISCC together with Cheat Sheets to recall the most important tools. The portal is constantly being expanded with new materials for different target groups, such as interdisciplinary users without affinity for computer science, beginners, advanced users and advanced software developers. Stay tuned to discover how the portal develops!

We appreciate your visit to our website here:

Announcement: European Trilinos & Kokkos User Group Meeting, 24.06.-26.06.2024 @HSU

The European Trilinos & Kokkos User Group (EuroTUG 2024) meeting will take place on the campus of the Helmut-Schmidt-University / University of the Federal Armed Forces Hamburg, in Hamburg Germany on 24.06.-26.06.2024. For the first time, the workshop further strives to bring together Kokkos users and developers in the same spirit. This will not only foster efforts in the European Kokkos community with regard to

scientific computing on heterogeneous hardware, but it will also leverage additional synergies between Trilinos and Kokkos developments. Participants can contribute to the formation of a vibrant European network, fostering collaboration among users and developers. Throughout the meeting, participants can anticipate a diverse program including introductory tutorials on Trilinos and Kokkos, talks by active developers, insightful presentations by engaged users, and group discussions covering relevant topics.

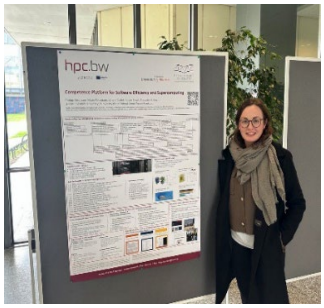
You can find more information on our website here:

Registration is open until 15.05.2024. You can register free of charge here:

CBRZ Power Supply

In January 2024 the CBRZ was connected to the final power supply. This concludes an important step towards finishing the construction of the CBRZ as envisioned, as the final power supply provides the needed support for extending the ISCC and HSUper in the future.
The planned installation of a secondary power supply to provide energy while the primary power supply may not function for longer than a minute is still in an early phase. In 2023 several different types of energy buffer or storages were examined.

hpc.bw @Day of Research, HSU, 26.03.2024



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The fourth Research Day took place at HSU, where hpc.bw presented a poster to inform researchers and interested visitors about the project structure, supported performance engineering projects, and the new HPC Portal. Moreover, an interdisciplinary exchange and networking took place.

Further information and the poster can be seen here:

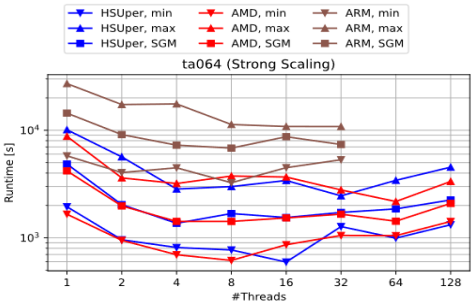
Visit from MissionLab Team

On 28.02.2024, hpc.bw staff met with representatives of the dtec.bw project MissionLab. After a tour to the CBRZ, Prof. Philipp Neumann and Prof. Oliver Rose gave presentations on high performance computing perspectives at HSU, computing topics in MissionLab and other research directions relevant to the research groups.

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 plot, a runtime comparison of the software Gurobi with various thread numbers and seed values for the benchmark ta064 (a time-dependent traveling salesman problem) is shown. Each hardware system (HSUper/Intel Xeon Platinum 8360Y, AMD EPYC 7763, ARM FX700) has a different color. Results are on the ARM sytem only computed up to 32 threads since this system has only 48 (physical) cores (and does not support hyperthreading). 10 different seed values are used for each thread number to take performance variability into consideration and each of these setups is computed three times. Hence, we show the runtimes as minimum, maximum and shifted geometric mean (with a shift value of 100) of the corresponding 30 (i.e., 3 runs times 10 seeds) computations.

The plot illustrates that a reasonable thread number is on all systems approximately in [4, 32]. Moreover, 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 identify the underlying hardware bottleneck(s). Are the performance differences only based on the clock speed and how about corresponding energy consumptions?



Outlook: hpc.bw @ISC 2024 & @Day of Armed Forces

We are proud to inform you that hpc.bw will be represented with a poster at the event of ISC High Performance. ISC connects industry users and technology developers and public in Hamburg from 12.05.-16.05.2024.

Moreover, there will be a comprehensive information levels at the Day of Armed Forces on the Campus of HSU at 08.06.2024. hpc.bw will not only be represented with a poster to learn more about the interdisciplinary project from our team members who will be present, but there will also be the opportunity to participate on HSUper tours to see the cluster from the inside and learn more about the implemented hardware.