



# Newsletter 04/2022

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 <a href="mailto:info-hpc-bw@hsu-hh.de">info-hpc-bw@hsu-hh.de</a>.

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## **Seminar Series Computation & Data in WT23**

In the winter trimester (WT 2023), 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.

#### Seminar sessions WT2023

Date	Room	Speakers	Title of lecture
26.01.2023; 14:30-16:00	H1, room 308	Chaitanya Kandekar (HSU)	A Thermo-hydro-mechanical modelling for concrete under fire loads
		Maria Krantz (HSU)	Generating Data for the Training of Machine Learning Algorithms for CPPS
23.02.2023; 14:30-16:00	H1, room 308	Nils Margenberg (HSU)	Hybrid Finite Element/Deep Neural Networks Methods for Accelerating Fluid-Dynamics Simulations
		Louis Viot (HSU)	New developments within the Macro/Micro Coupling software MaMiCo for highly parallelized multiscale flow simulation
30.03.2023 <b>14.30-16:00</b>	H1, room 308	Frederike Vogel (HSU)	Supervised learning for analyzing movement patterns in a virtual reality experiment
		Marcel Eckert (HSU)	How FPGAs can speed up algorithms by 2 examples

To subscribe to the seminar mailing list, send an e-mail to <a href="mailto:info-hpc-bw@hsu-hh.de">info-hpc-bw@hsu-hh.de</a>, subject line "Subscription Seminar Computation & Data". For more information, see: <a href="https://www.hsu-hh.de/wb/hpc-bw">https://www.hsu-hh.de/wb/hpc-bw</a>

## **Opening Ceremony for HSUper and CBRZ**



On 7 December, the hpc.bw team welcomed numerous visitors to the official inauguration of the supercomputer HSUper. After short opening messages by HSU president Prof. Dr. Beckmann, BMBF HPC project management representative Dr. Jochen Kerbusch, MEGWARE CTO Dr. Axel Auweter and Prof. Dr. Neumann (chair for HPC at HSU), HSUper was officially handed over to HSU. The visitors further had the chance to visit the container-based HPC computing center and to exchange on HPC, related technologies and applications during a reception.

Dr. Auweter and Prof. Dr. Neumann during the hand-over ceremony (Oulrike Schröder)

## Video on HSUper and CBRZ

A video presenting HSUper and the CBRZ is now available <u>here</u>. We thank MEGWARE, our PR department and the involved team for their support of the video production! Feel free to share the video with others!

## **New TOP500 Ranking for HSUper**

At the Supercomputing Conference, that was held Nov 13-18 2022 in Dallas/Texas, the new TOP500 list was presented. In the TOP10 computers, Italy placed its new system Leonardo which is ranked fourth, right after the Finnish machine LUMI. HSUper could mostly defend its spot in the lists, slightly slipping from rank 339 to rank 372 in the TOP500, from rank 98 to 102 in HPCG and from 71 to 80 in the Green500.

## **Update: HPC Competence Platform**

After the exchange about HPC competence areas, target groups and teaching-learning formats, the current focus of the work group "Competence Center hpc.bw" lies on website and software-sided realization. In particular, possibilities and limits need to be explored in order to develop an HPC Competence Platform implementation that is cross-target and promotes learning.

At the same time, we work on the content of the HPC Competence Platform. The aim here is to systematize existing learning content and to create own learning content. Existing offers such as the newsletter and the seminar series "Computation & Data WT23" will be incorporated.

# **Update: Performance Engineering Projects**

We currently work on two performance engineering tasks in the scope of the first call for performance engineering of the hpc.bw project.

The current primary task "Optimization of an IGA Code in MATLAB for parallel computing" has the aim to support Dr.—Ing. Georgios Michaloudis (Structural Analysis, UniBw M) in order to leverage the parallel computing capabilities of the in-house MATLAB Isogeometic Analysis Code. Current work focuses on performance profiling of the code to identify and subsequently improve performance-critical sections.

The second task "Enabling High-Throughput Studies of Reactive Materials" in collaboration with Univ.-Prof. Dr.-Ing. Denis Kramer (Chair of Computational Materials Design at HSU) has the purpose to improve workflows and compute-intensive parts thereof on HPC environments such as on our new cluster HSUper at HSU. Recent parallelization parameter explorations and the use of alternative solver configurations suggest potential performance improvements of up to 5% compared to previous parametrizations of the considered simulation benchmarks.

## **Closing Words for 2022**

An exciting year comes to an end: our supercomputer HSUper has entered service, first successful optimizations have been carried out in our performance engineering projects, the seminar series "Computation & Data" has entered the landscape of scientific exchange at HSU and UniBw M, a European Trilinos Workshop has been organized, just to name a few facts. And there is much more ahead: we have just started our collaborations on HPC and logistics this year, we strive to accomplish a scientific computing cloud for interactive use in education and research next year, the competence platform is taking shape these very days, and and

and 😌

With this I want to thank all hpc.bw members for the dedicating support and helping hands throughout this last year. Without you, HPC wouldn't be where it is now – so I am very much looking forward to what the new year will bring! I wish you all a merry Christmas and a good start into 2023!

Philipp Neumann

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**Chair for High Performance Computing**