Newsletter 02/2022

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 info-hpc-bw@hsu-hh.de.

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Update on the CBRZ

The technical establishment of our container-based high performance computing center (CBRZ) has been finalized to big extent: all the racks have been installed (see picture), challenges on power supply and network connectivity have been resolved, the final components of the machine have been delivered – we are thus soon ready to start a beta-user phase! Feel free to visit the CBRZ with our new supercomputer HSUper at the Open Campus (see below)!
The CBRZ was further already in the focus of a filming of a HSU image video on research and education.

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hpc.bw @ISC HPC

hpc.bw was represented at the congress ISC HPC, which took place 29 May to 2 June 2022 in Hamburg, in form of a project poster. We had several fruitful discussions on our development of the HPC competence platform, amongst others with representatives of the HLRN network as well as with establishers of the Hamburg HPC Competence Center and the international HPC certification program.
The picture to the right shows Piet Jarmatz, our representative of the HPC competence working group, in front of our poster.

© Piet Jarmatz

HSUper in the TOP500 List

On 30 May, the new TOP500 list of the fastest supercomputers worldwide (see also www.top500.org) was announced at the congress ISC HPC. Our new HPC cluster HSUper has entered the TOP500 list, ranked 339. In terms of German HPC systems, we are ranked 28. In terms of German sites (i.e., hosting institutions) with HPC, we are ranked 17. This is a very good result, since German sites that are ranked higher are mostly the "usual suspects", that is the sites of the Gauss Centre for Supercomputing and few centers of the newly established national high performance computing initiative (NHR).
There are two more lists that have been announced: the Green500, which measures the energy consumption, and the HPCG list which provides a measure for rather classical applications, such as sparse matrix-vector operations that are at the core of many numerical simulations. On HPCG, we are ranked 98 (rank no 13 in Germany), on Green500, we are ranked 71 (ranked 10 in Germany).

hpc.bw @ Open Campus

hpc.bw contributes to the program of the OpenCampus at HSU on 18 June. Feel free to drop by at our booth no. 42 in the HSU main building. Our umbrella project dtec.bw is represented at a booth closeby to which we also warmly invite you! In addition, we offer guided tours to our container-based high performance computing center (CBRZ) and the new supercomputer HSUper, which will take place right after lectures on “High Performance Computing@HSU: Numerical Simulation on 40.000 Compute Cores“ by Prof. Philipp Neumann, scheduled for 12:00 and 14:00. See the Open Campus website for more details on the entire program.

EuroTUG 2022 in Munich

The European Trilinos User Group Meeting will be held 12-14 September 2022 in Munich. The meeting, supported by hpc.bw to strengthen software sustainability, is organized by Dr. Matthias Mayr (UniBw M) and Dr. Alexander Heinlein (TU Delft). Click here for more details.

Collaborations

We are glad to welcome Opheo Solutions GmbH as collaboration partner in HPC. Our joint goal is to optimize and parallelize tour planning methods, which form a subclass of complex optimization problems. Addressing this endeavor requires insight from both the HPC and the application perspective. An actual kick-off for the collaboration is planned for this summer.

Performance Engineering Projects

In February 2022, the first call for support for performance engineering projects was published as part of the hpc.bw project. There were a total of eight applications. After going through a review process, carried out by the project coordinator and the hpc.bw multiplicators, four projects were accepted and are currently being jointly processed:

- Optimization of an IGA Code in MATLAB for parallel computing (Dr.–Ing. Georgios Michaloudis, UniBw M)
- Monte Carlo simulations of real fluids (Univ.-Prof. Dr.-Ing. Karsten Meier, HSU)

- Enabling high-throughput studies of reactive materials (Christopher Lange, HSU)
- benEFIT- Numerical simulation of non-destructive testing in concrete (Fabian Dethof, HSU)

Kick-off meetings with all groups have already taken place, and we look very much forward to these interdisciplinary software efficiency projects!

In addition, two projects in the area of service and consultation were adopted:

- C-STAR electric propulsion demonstrator multiphysics modeling (Maximilian Maigler, UniBw M; software installation and portability support to execute complex multi-physics simulations on HSUper)
- DigiTaKS* learning behavior of students in dealing with digital media and tools (Prof. Dr. Sabine Schmidt-Lauff and Dr. Therese Rosemann, HSU; continuous consultation and exchange on HPC and data analysis for student evaluation data on their digital learning behavior)

Further information on the projects and the cooperation with hpc.bw can be found at the following link: **https://www.hsu-hh.de/wb/hpc-bw**

Seminar Computation & Data

The seminar series Computation & Data started on March 31, 2022 with lectures by Yannis Schumann (Data-driven Inference of Stencils for Discrete Differential Operators) and Henrik Steude (It's more than a "model.train()" -- Modern Tools and Architectures for ML Systems). In April, Jens Bartnitzek from A+S Consult GmbH, who contributes to the dtec.bw project SHM, gave a presentation on "Infrastructure Information Modeling: workflow for an overall model infrastructure embedded in spatial base data". In June, we welcomed our international guest Derek Groen (Brunel University London), who presented his contributions to "Multiscale Migration Modelling using Supercomputers: enabling agent-based modeling forecasts in a world of messy, inaccessible, biased and incomplete data".

The next seminar session will take place on 30 June, 15:00-16:00, at HSU, lecture hall 3 (hybrid format via MS teams). Talks are planned by Benedikt Hein from the chair Technology of Logistics Systems/Prof. Kirchheim and by a representative of the dtec.bw project DS2CCP which aims at the development of a digital sensor-2-cloud campus platform, headed by Prof. Scholl.

If you are interested in joining the seminar's mailing list, please send an e-mail to info-hpc-bw@hsu-hh.de with the subject line „Subscription Seminar Computation & Data".

Update: Work Group „Competence Center hpc.bw"

The work group "Competence Center hpc.bw" strives to develop ideas on the structure, concepts and educational components of a to-be-established competence center on HPC. In this scope, a building block concept was developed to combine interdisciplinary expertise and experience. Due to its flexible use, it can be applied in situation-specific contexts performed as stand-alone units, as well as in individual combination.

Currently, the work group addresses:

- the deepening and discussion of contents as well as development of first prototypical building block-based concepts,
- the discussion on target group-specific suitability of certain teaching-learning formats and

competence areas,

- the development of scenarios for possible activities.

The four categories that need to be integrated to form a specific action target in the competence platform are shown below and have been discussed with the hpc.bw consortium and with internationally recognized experts at the conference ISC HPC.

For open questions and interdisciplinary exchange, the work group is available via the following email address: jessica.kleinschmidt@hsu-hh.de

Target Group / Participants				HPC Competence Areas		Basic Implementation Form	Learning-teaching and Overarching Formats Conference, Project Weeks, Podcast etc.		
Interdisciplinary Users without an Affinity for Computer Science	Beginners	Advanced Users	Advanced Software Developers	Technical Competences	Meta Competences		Teaching of Competences	Discussion & Exchange	HPC Consulting
Without an affinity for computational processes Only write individual lines of code or have no experience with HPC, programming or optimizing software	Basic knowledge of computer science Have scientific question which can be to tackled through HPC exists Write parts of programmes, e.g. larger Excel macros, MATLAB scripts or interfaces for commercial software	Intermediate knowledge of computer science Advanced knowledge (write their own programmes / parts of programmes for parallelized execution on HPC systems)	Comprehensive knowledge of computer science Parallelize and optimize software largely independently and have detailed knowledge of job scheduling systems such as SLURM or PBS	Fundamental HPC knowledge	Existence of HPC and awareness of the existing possibilities	**On-site**	Workshop	Barcamp	Office hours
				Using commercial software	**Understanding error messages**	Digital	Seminar	Review-meetings	Helpdesk
				Using HPC systems independently	Informal learning (through curiosity that nessecitates situation-specific trial and error)	**Blended learning**	Lecture / ring lecture	**Meet-up**	Sharing written instructions / videos
				Software Engineering	**Resilience at work**	**Hybrid**	Tools-talk	Poster presentations	Infopoint
				Visualisation	Understanding and using manuals		Training	Colloquium	Sharing of contact partners
				Performance Engineering	Informed internet research		Own videos	Podium discussion	Professional discussion on equal level
					Tactics for solving technical problems and systematic root cause analysis		**Learning material / wiki / tutorial / PDF**		Technical support (advanced consulting)

Notes: Colored matches are based on experiences and interests of the hpc.bw team. However, all combinations are possible.
White boxes could be applied in all target groups.