Newsletter 02/2023

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.

Contents

Seminar Series Computation & Data in HT23

In the autumn trimester (HT 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 (coordinates will be provided at a later stage), it is also possible to participate digitally via MS Teams.

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.

| Date	Presenter	Titel
25.10.2023	Maria Maleshkova	Digital Twins – Building Blocks for Medical Data Science
	Thomas Carraro	The HiBRAIN project: Combined data- and model-based design of lithium-ion battery electrodes using artificial intelligence
29.11.2023	Therese Rosemann & Yannis Schumann	Digital Competences and Digital Learning Behavior in Higher Education - Generation of individualized Feedback in a Longitudinal Study (DigiTaKS* and hpc.bw)
	Sergej Grednev	Prediction of Structure-Property Relationships in Cellular Materials
13.12.2023	Maximilian Maigler	Coupled PIC-DSMC and Molecular Dynamics Modeling of Radio Frequency Gridded Ion Thruster Erosion
	Valentina Pessina	Modeling Rarefied and Continuous High Angle-of-Attack Hypersonic Reentry into Martian Atmosphere with Open-Source Software

New HPCCP Website Online

We are very pleased to announce that the website for our HPC competence platform (HPCCP) is online!
On the website you will find all important information about hpc.bw. In addition to a brief introduction of the interdisciplinary consortium from different chairs at HSU/UniBw H and UniBw M, you will also see an archive with past newsletters about activities in the project. Furthermore, we share insights into the manifold projects related to Performance Engineering, which are supported by hpc.bw. The short presentation of the projects gives you an overview into the variety of research possibilities with HPC and the supercomputer HSUper. Last but not least, the HPCCP website also displays the latest news on research and public relations activities as well as the upcoming events. In order to keep abreast about the seminar series Computation & Data, HPC user meetings and other events, check our event calander.

Feel invited to visit our new website here or scan the QR-code:

Continuing Work on the HPC Competence Platform Contents
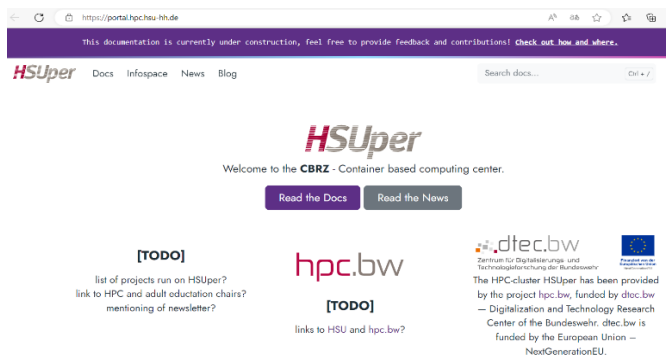
©Marie Rathmann

The hpc.bw team continues to work intensively on contents of the HPC competence platform.

Different formats such as cheat-sheets, workshops, open educational resources, seminar series, etc. are to be used to promote competence, knowledge transfer as well as discussion & exchange and HPC consulting. In terms of content, the formats on the competence platform reflect the diversity of HPC. On the one hand, this includes basic HPC knowledge, independent use of HPC systems and software engineering. On the other hand, there is also the awareness of the existing possibilities of HPC, the understanding and use of manuals as well as tactics for solving technical problems. These formats are to be delivered in a variety of ways, such as purely digital on the platform and in hybrid form, but also as blended learning and on-site.

HSUper Workshop, 28.09.2023

As part of the HPC competence platform, a HSUper workshop will be held at the HSU on 28.09.2023. The workshop is aimed at beginners and advanced HPC users. We cordially invite you to attend the workshop to gain a comprehensive insight into High Performance Computing and an introduction to the use of the HSUper supercomputer!
Topics such as HPC and Linux basics, data transfer to HSUper, obtaining hardware information and utilizing the BeeGFS parallel storage system will be covered. In addition, the workshop will provide information on how to use module systems, install and load software packages. Besides an introduction on how to allocate nodes of HSUper interactively or by writing scripts, forwarding the output of graphical applications with X11 is also covered. The contents will be demonstrated with practical examples. We also offer a tour of HSUper. You are cordially invited to attend the HSUper workshop if you are interested in learning more about HPC and how to perform computations on HSUper, or if you already have some experience working with this super computer!
Please register for the workshop until 14.09.2023 by sending an e-mail with subject line "Registration: HSU-per workshop 28.09.2023" to workshops-hpc-bw@hsu-hh.de.

Scan the QR-Code or click here to have a look into the schedule of the workshop:

Interactive Scientific Computing Cloud (ISCC): Test Phase Ahead!

The Interactive Scientific Computing Cloud aims to fill the gap for users with specific needs that cannot be containerized as well as users with workloads that cannot be satisfied by existing local machines and do not yet require the entire power of HSUper. This cloud solution also aims to lower the entry barrier for new users as the guest operating system can be chosen.

Another use case is to take advantage of the faster connection to HSUper file systems (compared to computers on campus) and use remote desktop connections to a virtual machine for data-intensive post- or preprocessing steps that would normally be performed on local machines rather than on an HPC system.

The ISCC consists of 10 nodes with the same hardware specifications as HSUper, except for the Interconnect, which is capable of 50Gb/s over Ethernet instead of InfiniBand HDR100. There are also two nodes with 1TB of memory and 8 NVIDIA A30 GPUs. Each of these GPUs can be split into virtual GPUs and assigned to different virtual machines.

The alpha test phase has just started and the beta test phase will start in July. Please email us if you are interested in testing the new platform with us: info-hpc-bw@hsu-hh.de

New Faces: Alexander Kolling und Marie Rathmann

We welcome two new faces to the project: Alexander Kolling and Marie Rathmann have been supporting the hpc.bw project since May 2023.
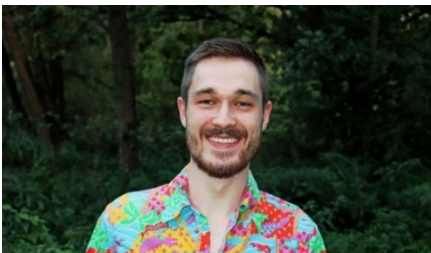
©Alexander Kolling

Alexander Kolling is responsible for the digital HPC competence platform. The platform will provide wide information about HPC in general, HPC-related projects and the HPC cluster HSUper at HSU. The main task for Alexander Kolling is to collect and prepare all necessary information and design a digital educational environment for various target groups. He is also going to create modularized online courses and educational resources with open accessibility.

Marie Rathmann is responsible for the organisational aspects of the hpc.bw project, such as events, the seminar series Computation & Data as well as making the project visible to the public and so on. She also supports the growth of HPC competence platform with regard to the processing of HPC content from an adult education perspective.

©Marie Rathmann

hpc.bw @ Open Campus 2023

HPC.bw as well as the supercomputer were presented at this year's Open Campus on 24.06.2023. The project was represented both in the umbrella organization dtec.bw with a poster and with its own booth, at which visitors informed themselves about high performance computing.

©Marie Rathmann

In addition, Prof. Philipp Neumann gave two lightning talks, in which participants were introduced to HPC in general, respective research at HSU and to the supercomputer HSUper. The latter could be visited right after the talks (HPC-Cluster tour).

Here you can find the related article on our website and the presented poster:

hpc.bw @ Day of Adult Education at University Mainz

At the Day of Adult Education on 23.06.2023 at the University of Mainz, the hpc.bw project was presented with a poster. At the so-called Market of Opportunities, many interested scientists and practitioners from the field of adult education and further education informed themselves about the competence platform for high performance computing as well as the supercomputer.

Here you can see the associated article and the poster:

©Marie Rathmann

Project Update: Performance Engineering for an Isogeometric Analysis Code

We wrapped up our work on the performance engineering project "Optimization of an IGA Code in MATLAB". We found that substantial sequential time-savings could be achieved by rigorously adapting vectorization in the procedures used to construct element-wise stiffness matrices. This was only shown on an excerpt due to time constraints. Investigations into the use of "parfor"-parallelization and its alternatives showed that further work is needed on scalable parallelization practices for FEM Matlab-code.

Project Update: Logistics and Optimization
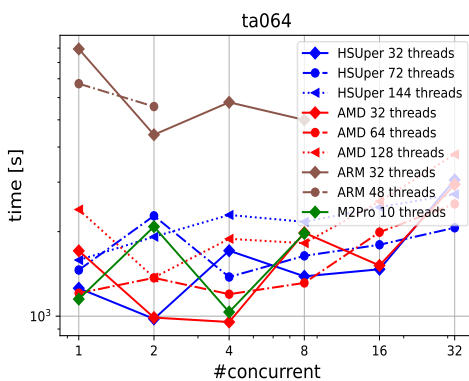
©Willi Leinen

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 (considering both shared memory multi-core parallelization as well as distributed computing). Recently, we experimented with the concurrent optimization feature of the software Gurobi and an M2 Pro chip. In the figure, a performance experiment of the benchmark ta064, a time-dependent traveling salesman problem, is shown. The default settings (10 threads on M2 Pro, 32 threads on the other machines, and 1 concurrent instance) often lead to good results. However, the smallest computation times are often achieved with 2 or 4 concurrent instances. More work is to be conducted on more test cases and distributed computing.

4

Project Update: Understanding Opheo Performance

In recent work, we have been focussing on code metrics and documentation to ensure a comprehensive understanding of the performance of the ixOptimizer, an optimization software developed by Opheo Solutions GmbH for logistics (tour planning). Our analysis has involved examining the initial code and identifying the key data structures, classes, and modules associated with the ixOptimizer. Additionally, we have been closely examining the main functions called within the ixOptimizer to gain insights into its behavior and to identify any potential bottlenecks. Concurrently, we have been conducting an operator study, reviewing the most commonly used operators to identify more optimal routes. Our aim is to optimize the code by merging certain operators, thereby reducing the total number of operators employed. This approach will be further evaluated through new benchmarks, which will allow us to compare the performance of the updated approach with the existing one. Overall, these efforts contribute to improving the efficiency and maintainability of our project.