Newsletter 03/2022

Newsletter

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 HT22

In the autumn trimester (HT 2022), 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.

Date	Room	Speakers	Title of lecture
27.10.2022; 14:30-16:00	H1, room 205	Andreas Fink *(HSU)*	HPC for Solving Combinatorial Optimization Problems in Logistics: Challenges and Examples
		Benedikt Hein *(HSU)*	Distributed Deep Reinforcement Learning: How a hundred years of experience can be gathered in one day
09.11.2022 11:00-12:00	Aula, room 2	Matthias Mayr *(Universität der Bundeswehr München)*	Sustainable development of multi-level block preconditioners in Trilinos/MueLu
24.11.2022 14:30-16:00	H1, room 205	Gary S. Schaal *(HSU)*	N.N.
		Alexander Popp *(Universität der Bundeswehr München)*	Scalable computational kernels and linear solvers for FEM-based computational contact mechanics
15.12.2022 14.30-16:00	H1, room 205	Bernd Flemisch *(Universität Stuttgart)*	The open-source simulator DuMux - experiences and practices from 15 years of development
		Powei Huang *(Eidgenössische Technische Hochschule Zürich)*	Reactive transport modeling in aqueous environments using the Nernst-Planck formulation

For registration please send an e-mail to info-hpc-bw@hsu-hh.de with the subject line „Subscription Seminar Computation & Data”. For more information, see: https://www.hsu-hh.de/wb/hpc-bw

hpc.bw @ Open Campus HSU

On 18 June 2022, the team welcomed numerous visitors to the Open Campus at the hpc.bw booth. In addition, visitors could learn more about HPC at the presentation “High Performance Computing: Numerical Simulation on 40.000 cores”. The High Performance Computing (HPC) - Cluster Tour made it possible to visit the CBRZ with its supercomputer HSUper and see it in action.

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Kick-off with Opheo Solutions

On 20 July, a kick-off meeting was held between representatives of HSU and Opheo Solutions GmbH to discuss joint work on optimizing and parallelizing the tour planning software. First steps in this direction are being taken, we look very much forward to the collaborative project!

hpc.bw @ (Aus)Bildungskongress der Bundeswehr (Educational congress of the federal armed forces)

From 13 to 15 September 2022, the Education congress of the federal armed forces took place at the HSU. The hpc.bw project participated in the poster exhibition of the dtec.bw projects at the HSU.

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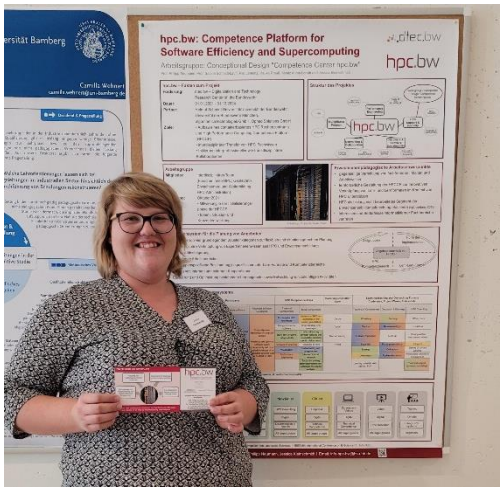
hpc.bw wins 3rd place at the wbv poster award



Our colleague Jessica Kleinschmidt received the third wbv Poster Award for the poster "hpc.bw: Competence Platform for Software Efficiency and Supercomputing". The wbv poster award was given at the Section Conference on Adult Education of the German Society for Educational Sciences (DGfE) in Flensburg. We congratulate Jessica to this success and look forward to even more synergies during the establishment of the HPC competence platform!

Link to the press release:
https://www.wbv.de/fileadmin/webshop/pdf/2022-09_16_Pressemitteilung_Posterpreis-%20DGfE_2022_FINAL.pdf
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EuroTUG 2022 at UniBw M

©The Trilinos Project

This year's European Trilinos User Group (EuroTUG) meeting took place on September 12 - 14, 2022. After a pause of three years, the EuroTUG 2022 offered an interactive forum for Europe-based users and developers of the Trilinos project. The participation of 29 researchers from various European universities as well as Trilinos core developers from Sandia National Laboratories made this community workshop a complete success.
On the first day, the workshop started with a tutorial session, such that new Trilinos users could take their first steps in building and using the Trilinos software stack under the guidance of experienced Trilinos developers. These hands-on tutorial sessions attracted a number of researchers from research groups across Europe and have been described as "insightful and inspiring" by many of the participants. The second and third day offered five user presentations, where Trilinos users reported on their integration of Trilinos in application codes and shared their experience with Trilinos in day-to-day research. The program was complemented by a five developer talks, where Trilinos core developers from Sandia National Laboratories told the community about recent achievements, new features and future developments in the different product areas of Trilinos. Each day also included roundtable discussions among all participants to exchange their view on topics such as:

- Lifecycle model in Trilinos and application codes: how to organize refactoring and new versions?
- Containerization & virtualization: which approach is best for which use case / workload? How to setup Trilinos quickly on a new machine?
- How to structure collaboration across Europe and with Sandia National Laboratories?
- Trends in using GPUs and other high concurrency nodes in the European community.

As the highlight of EuroTUG 2022, Mike Heroux (Director of Software Technology, US DOE Exascale Computing Project) delivered a keynote lecture entitled "Leadership Scientific Software Trends from 2000 – 2040 through the Lens of the Trilinos Project", where he shared his view and vision for scientific computing software ecosystems for the next decades.
EuroTUG 2022 has been organized under the auspices of the Center for Digitization and Technology Research of the Bundeswehr (dtec.bw) and has been embedded into the project “hpc.bw – Competence Platform for High Performance Computing” of dtec.bw. The workshop has been organized by Dr. Matthias Mayr (UniBw M) and Dr. Alexander Heinlein (TU Delft).
Although this year's EuroTUG has just finished, we're already looking forward next year, where the meeting will be held at TU Delft.

HSUper enters production

We are glad to inform you that, after some weeks of beta testing, our supercomputer HSUper is now ready and enters the production phase. Documentation of the machine and its use can be found at https://www.hsu-hh.de/hpc/en/hsuper/ which includes, amongst others, information on available modules and software as well as exemplary job submission scripts (the scheduling is performed with SLURM) including test codes. Some outtakes of the general information is provided in the following.
Different SLURM partitions are provided for various use cases:

- dev: jobs on 1-2 nodes and a wall-clock limit of 1h (use this partition for testing purposes only!)
- small: jobs running on 1-5 regular compute nodes with a wall-clock limit of 72h and exclusive node reservation

- small_shared: same as small, but nodes are by default shared with other applications. This makes particularly sense for applications that require (multiple) jobs with low core count and memory demands. E.g., running a simulation under 9 different parametrizations with each simulation using 8 compute cores can leverage a single compute node in this setting
- small_fat: running on 1-5 fat memory nodes with a wall-clock limit of 24h and exclusive node reservation
- small_gpu: running on 1-5 GPU nodes with a wall-clock limit of 24h and shared node reservation by default; use the SLURM parameter "--exclusive" in your job scripts to switch to exclusive use
- medium: jobs on 6-256 regular nodes with a wall-clock limit of 24h and exclusive node reservation
- large: jobs on more than 256 nodes (available to selected users upon request only!)

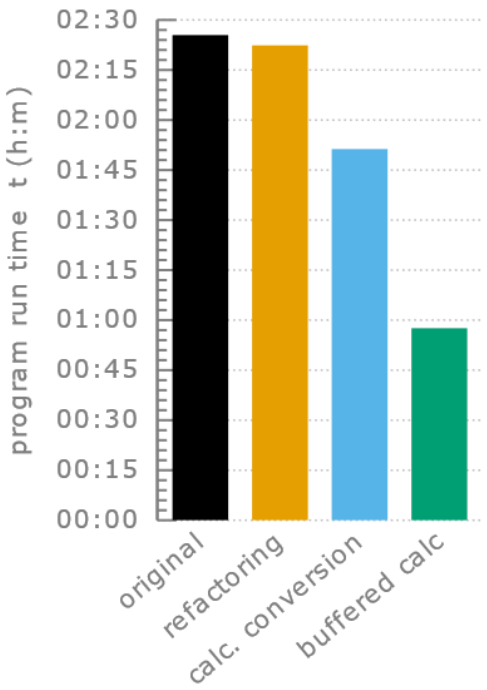
HSUper has been brought to life by support from dtec.bw. Therefore, users are asked to acknowledge HSUper use in their respective scientific contributions such as papers.
In case of questions, feel free to contact the CBRZ and HSUper staff via info-cbrz@hsu-hh.de.

Performance Engineering Project - "Monte Carlo simulations of real fluids"

The project "Monte Carlo simulations of real fluids", in collaboration with Univ.-Prof. Dr.-Ing. Karsten Meier (Chair of Thermodynamics at HSU), is one out of four projects supported in the scope of the first call for performance engineering of the hpc.bw project.

It aims to reduce the runtime of a molecular dynamics (MD) simulation research program. The bar chart visualizes the run time of four exemplary implementations of the MD simulation.

First, an identification of bottlenecks, their isolation into subroutines (refactoring) and a conversion of their respective calculation structure have been carried out (calc. conversion). Finally, these routines have been re-implemented and extended, in particular, to leverage SIMD (single instruction multiple data) instructions. These measures reduced the program runtime for the examined test case by over 50% (buffered calc).



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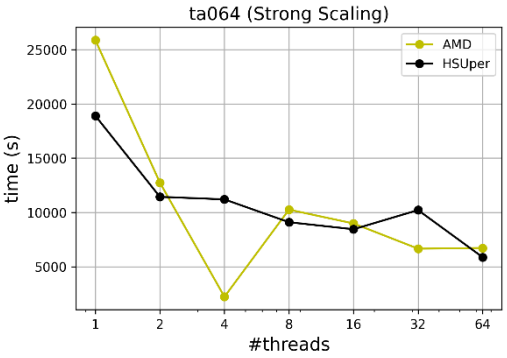
hpc.bw@HPC for Logistics

While HPC is already well established in research and development fields such as engineering and science, there is still much room for solving optimization problems in business administration and economics. Existing optimization methods often have a sequential flow logic at their core (with limited data-parallel concurrency), which is why such algorithms often must be adapted or even newly designed and implemented for HPC architectures with parallelization in mind.



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In a first step, we are 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). The above graph shows first scalability experiments using the software CPLEX on the time-dependent traveling salesman problem for the benchmark graph configuration ta064[1], leveraging AMD EPYC 7763 and Intel 8360Y processors; the latter corresponds to the hardware that is used in our supercomputer HSUper.

[1] A. Fink, S. Voß. European Journal of Operational Research 151(2):400-414, 2003