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Newsletter 01/2023

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.

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Seminar Series Computation & Data in FT23

In the spring trimester (FT 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.

The next talks will be given on 27 April 2023, 14:30-16:00, in room 113-115, container building C2/S2 (near Grandplatz):

Philipp Marienhagen: **Calculation of equation-of-state data in many-particle systems consisting of hard-anisotropic particles**

Yannis Schumann: **Distinguishing Molecular Tumor Subgroups Using Deep Learning**

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.

New Performance Engineering Projects Supported by hpc.bw

On 14 February 2023, the application period for performance engineering project proposals finished. All in all, five proposals were submitted: one proposal from UniBw Munich and four proposals from HSU, with the latter all originating from the faculty of economics and social sciences. After careful review and discussion, three projects have been selected for hpc.bw performance engineering:

Wittenberg, Philipp	HSU	HPC for semi-parametric statistical modeling on massive data sets
Wiedra, Frank	HSU	Personnel scheduling in roll-on/roll-off-terminals (RoRo-terminals)
Mayr, Matthias	UniBw Munich	Performance portability for the MIRCO BEM solver for rough surface contact

The other two projects will be supported by hpc.bw through code inspection and programming consultation:

Hipp, Andreas	HSU	The 2-stage no-wait hybrid flow shop scheduling problem
Hipp, Andreas	HSU	Single machine scheduling with position dependent maintenance

The projects are to be carried out from April 2023 – March 2024. The hpc.bw team looks forward to these interdisciplinary activities.

Workshop with Bundeswehr

On 8 March 2023, hpc.bw organized a workshop with members of the Bundeswehr at UniBw Munich to exchange on needs and potential collaborations in the field of high performance computing. After a short welcome (Prof. Alexander Popp), a brief introduction to dtec.bw (Mr. Klaus Wangelin) and an overview of hpc.bw activities (Prof. Philipp Neumann, Dr. Matthias Mayr), the participants of Bundeswehr presented their work field and related computing

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challenges. We thank all participants for the stimulating discussions and look much forward to fostering more exchange in the future!

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 (considering both shared memory multi-core parallelization as well as distributed computing).

Recently, we ported the software Gurobi to these systems and the ARM Fujitsu PRIMEHPC FX700 platform. In the figure, a scalability experiment of the bench-

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mark ta064, a time-dependent traveling salesman problem, is shown. Speedups could be observed for this case especially on the AMD and Intel (i.e., HSUper) systems using up to 16 threads. More work is to be conducted on more test cases and different parallelization options.
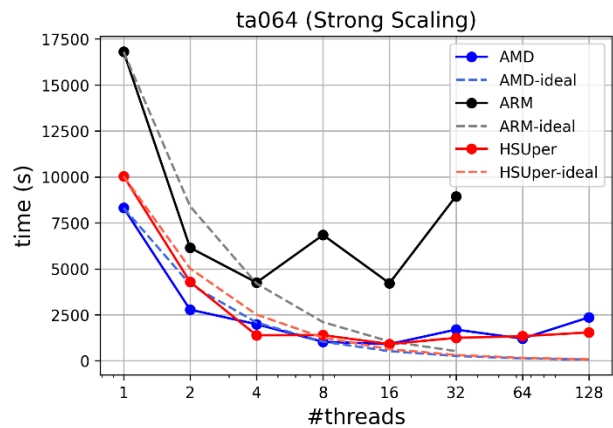
Project Update: Performance Engineering for an Isogeometric Analysis Code

We are in the process of wrapping up the task "Optimization of an IGA Code in MATLAB". Some points studied during this project where MEX routines, `parfor`- and `spmd`-parallelization and profiling in general. Minor changes to the code where able to reduce the program runtime by up to 5%. Rigorous administration of such changes to further spots could increase those savings further. We currently investigate the application of distributed array data structures and their realization inside the IGA software.