Erlangen National High Performance Computing Center

Newsletter #5

December 2021

In This Issue...

Quick News

Dr. Bandwidth in the NHR PerfLab Seminar

On Wednesday, December 15 at 4:00 p.m., John D. McCalpin (a.k.a. "Dr. Bandwidth"), the developer of the famous STREAM benchmark, will give a talk on "Memory Bandwidth and System Balance in HPC Systems." Details at: hpc.fau.de/?p=10231

LIKWID Bugfix Release

LIKWID 5.2.1 is out! This is mainly a bugfix release, albeit an important one. For example, it fixes issues with counter multiplexing when using the Linux *perf* backend. Read the details at: hpc.fau.de/?p=10266

Newsletter mailing list

You can now subscribe to a mailing list in order to get notified when a new NHR@FAU newsletter is out: lists.fau.de/cgi-bin/listinfo/nhr-newsletter

Missed a talk?

The NHR@FAU YouTube channel at youtube.com/NHRFAU provides recordings of some talks, lectures, and courses, as far as this is covered by copyright restrictions.

Atomistic Simulation Center Virtual Inauguration Symposium

The three NHR centers in Berlin, Paderborn, and Erlangen are united by their thematic focus on simulations of complex atomic and molecular systems. The establishment of the *NHR Atomistic Simulation Center* (ASC) was therefore a natural step and was presented to the scientific community through a virtual opening symposium on October 25 and 27. After a welcome address by FAU Vice President Prof. Dr. Georg Schett and an introduction to the NHR concept by NHR@FAU Director Prof. Dr. Gerhard Wellein, seven invited speakers and as many representatives of the ASC provided updates on current aspects and challenges of atomistic simulations using high-performance computing. Topics such as advanced materials, soft matter, life science, quantum chemistry, and algorithms were at the focus of the individual sessions. With nearly 300 registrations, the event was a resounding success. It thus helped tremendously to promote the NHR network, and especially NHR@FAU, in the community. More information at: tiny.cc/ASC-NHR-2021

"Alex" Cluster Friendly User Phase

Alex is the Tier-3 and NHR GPGPU cluster with Nvidia A100 and A40 accelerators at NHR@FAU. The hardware of Alex has been delivered in November. It is currently running "friendly user" workload in order to weed out performance problems and bad hardware. Early adopters are working closely with the HPC team to optimize system configuration and installed software. This phase is planned to end by early February.

NHR Centers Accepting Project Proposals

The NHR Association is in the process of establishing a central application portal and a common process for project proposals by scientists with significant need for compute cycles at Tier 2. In the meantime, it is still possible to apply for compute time at each center directly. Details can be found at www.nhr-gs.de/ueber-uns/nhr-verein. Since the installation of the first NHR cluster at NHR@FAU is still ongoing, a pre-registration form is available at hpc.fau.de/nhr-vormerkliste/.

First European Master's Degree Program in HPC

A European consortium including FAU aims to develop a pan-European pilot Master's degree program for high performance computing. As of the winter term 2022/23, the partners plan to provide courses that will offer students excellent career opportunities in the rapidly-growing fields of HPC and high-performance data analytics. The program will focus on areas such as design, application, operation, and use of current and future generations of HPC and HPC-related technologies in Europe. It will also provide training to experts who are capable of driving forward the introduction of HPC and the transfer of knowledge in industry and at universities. More information at: hpc.fau.de/?p=10180

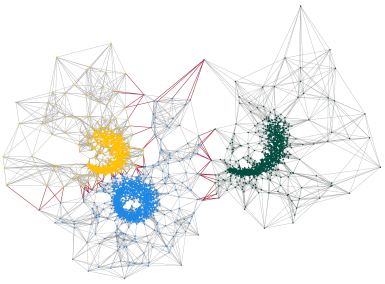
Recent Events

From October 11–13, Thomas Gruber, Jan Eitzinger, and Georg Hager from NHR@FAU conducted a special version of the popular *Node-Level Performance Engineering* tutorial targeted at experienced performance engineers from other NHR centers. The teaching material was thoroughly discussed among the instructors and the 16 attendees, including background knowledge and pedagogical issues. This was our first take at *train-the-trainer* events, which will ultimately empower attendees to conduct similar courses on their own, using the material provided.

LRZ Garching, Intel, and NHR@FAU conducted the online *PRACE HPC Code Optimisation Workshop 2021* from November 2–4. In this course, about 45 attendees developed an awareness of the features of multi- and manycore architecture that are crucial for modern, portable, and efficient applications. Thomas Gruber from NHR@FAU was responsible for the LIKWID hands-on exercises. Gerald Mathias from LRZ reported on optimizations in the popular molecular dynamics code *CPMD*, which were mainly developed by Tobias Klöffel from NHR@FAU.

Establishing an active community involves regular communication among its members. To this end, the competence network for scientific high-performance computing in Bavaria (KONWIHR) organizes regular welcome workshops for its new projects to discuss their planned work with fellow KONWIHR members and HPC experts from RRZE and LRZ. In the latest workshop on October 11, topics included implementation of new methods for parallel molecular dynamics simulations using LAMMPS (Prof. Zahn, FAU), improving finite-element algorithms for coupled multiphysics problems and non-matching grids (Prof. Wall, TUM) and optimizations of large-scale simulations of induced earthquakes (Prof. Bader, TUM). Additionally, researchers from the University of Würzburg (Prof. Assaad, Dr. Goth) reported on their ongoing efforts of disseminating domain-specific as well as more general HPC knowledge at their university and beyond.

December Highlight: Multiway *p*-Spectral Clustering



Clustering is the act of segmenting a set of data into several groups, with the aim of obtaining parts of roughly equal size with strong internal and weak external connections. It is used in many scientific fields including pattern recognition, bioinformatics, and machine learning. Spectral clustering is a widely used method that can be applied to any kind of data with a suitable similarity metric between them forming a graphical structure. It takes advantage of the information present in the eigenvectors of the *graph Laplacian*, a matrix representation of the graph, in order to obtain discrete partitions. Researchers at USI Lugano (Switzerland) and NHR@FAU have collaborated to develop an algorithm that improves the quality of spectral clustering by using sharper p-norms and multiple eigenvectors to compute the clusters. For more details, see the paper by Dimosthenis Pasadakis, Christie Louis Alappat, Olaf Schenk, and Gerhard Wellein in the journal *Machine Learning* at: DOI:10.1007/s10994-021-06108-1

FAQ Corner: CPUs

Is it true that Arm processors are now competitive in HPC?

"Arm CPU" just means that it uses an instruction set architecture (ISA) licensed from Arm, but the hardware implementation can vary a lot. There is a plethora of Arm-based designs, some from Arm and many from other vendors. Many target the low-power/embedded market, but there are some which have entered the HPC area. Prominent examples are the Fujitsu A64FX and the Marvell ThunderX2. A TX2 system is available in the NHR@FAU test and benchmark cluster.

I heard that RISC-V is "the new thing."

RISC-V is just a modern, open instruction set architecture (ISA) that does not have the licensing issues of Arm. However, the underlying processor architecture will mainly determine the performance of code. So far, competitive RISC-V designs are nowhere to be seen in HPC, but this may change in the future.

What is a vector computer?

A vector computer has an ISA and CPU architecture that enable efficient operations on array data. This goes under the name of *Single Instruction Multiple Data* (SIMD). SIMD features have proliferated in commodity CPUs as well, but a true vector CPU has features that make it more efficient, such as large vector lengths (e.g., 256 elements) and a high memory bandwidth (e.g., 1.5 Tbyte/s). Currently, only NEC offers a true vector processor, the *SX-Aurora Tsubasa*. A node with two Tsubasa cards is available in the NHR@FAU test and benchmark cluster.

What about the Apple M1?

It's positively impressive, in terms of memory bandwidth as well as the architecture of its memory hierarchy. Current models still lack the peak performance needed to be competitive with x86 server CPUs, however.

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NHR newsletters

Spotlight: Dr. Georg Hager

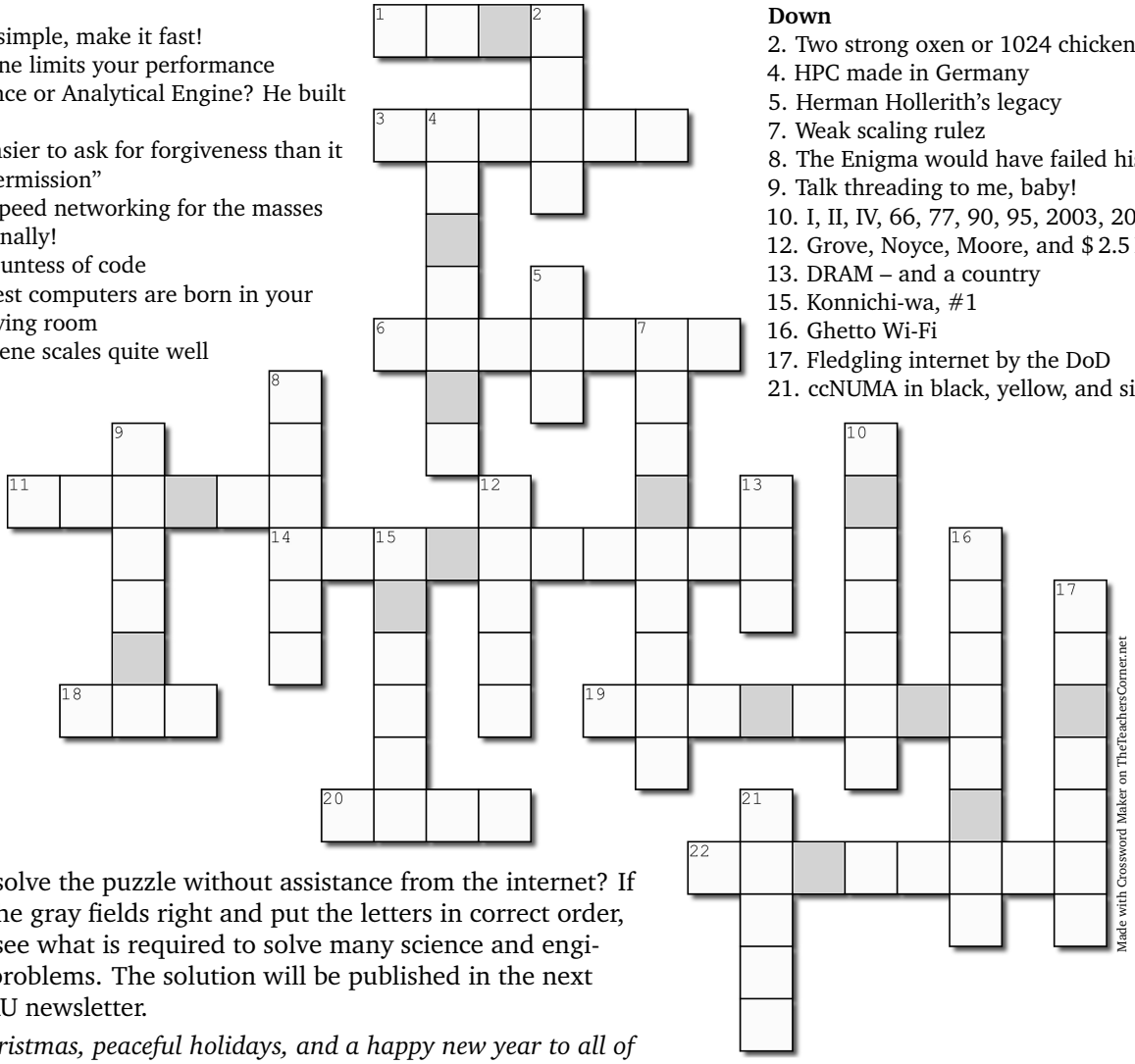
Georg Hager holds a PhD and a Habilitation degree in Computational Physics from the University of Greifswald. He leads the Training & Support Division at NHR@FAU and is an associate lecturer at the Institute of Physics at the University of Greifswald. Recent research includes architecture-specific optimization strategies for current microprocessors, performance engineering from core to system level, and the analytic modeling of structure formation in large-scale parallel codes. At NHR@FAU he is responsible for organizing the training and event program and for orchestrating collaborative performance engineering activities.

In his spare time, he maintains a collection of old computing devices, especially programmable calculators from the 1970s and 1980s and slide rules. This goes well with his interest for computer history and electronics tinkering. Georg is married with two grown-up kids.

HPC and Computer History Crossword Puzzle

Across
1. Keep it simple, make it fast!
3. This Gene limits your performance
6. Difference or Analytical Engine? He built neither
11. "It's easier to ask for forgiveness than it is to get permission"
14. High-speed networking for the masses
18. 4.0! Finally!
19. The countess of code
20. The best computers are born in your parents' living room
22. This Gene scales quite well

Down
2. Two strong oxen or 1024 chickens?
4. HPC made in Germany
5. Herman Hollerith's legacy
7. Weak scaling rulez
8. The Enigma would have failed his test
9. Talk threading to me, baby!
10. I, II, IV, 66, 77, 90, 95, 2003, 2008, 2018
12. Grove, Noyce, Moore, and $ 2.5 M
13. DRAM – and a country
15. Konnichi-wa, #1
16. Ghetto Wi-Fi
17. Fledgling internet by the DoD
21. ccNUMA in black, yellow, and silver



Can you solve the puzzle without assistance from the internet? If you get the gray fields right and put the letters in correct order, you will see what is required to solve many science and engineering problems. The solution will be published in the next NHR@FAU newsletter.

Merry Christmas, peaceful holidays, and a happy new year to all of you!