NHR FAU

Erlangen National High Performance Computing Center

Newsletter #7

April 2022

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Quick News

Talk on OpenMP offloading in PerfLab seminar

Christian Terboven from RWTH Aachen will give an introduction to OpenMP accelerator directives on April 5. Details at: hpc.fau.de/?p=10069.

Talk on `gprofng` in PerfLab Seminar

Ruud van der Pas of OpenMP fame will speak about the new `gprofng` profiling tool on April 12. See hpc.fau.de/?p=11404 for details.

HPC Café on SLURM

On April 12 at 4 p.m., the monthly HPC Café will focus on best practices with the SLURM batch scheduler.

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.

NVIDIA DLI Ambassador at NHR@FAU

We are proud to announce that NHR@FAU now has an NVIDIA Deep Learning Institute (DLI) Ambassador. NVIDIA certifies qualified educators to deliver the latest hands-on workshops free for university faculty, students, and researchers in the areas of GPU-accelerated computing, AI, and data science. Dr. Sebastian Kuckuk, an NHR liaison scientist with the Chair for System Simulation (LSS), has successfully passed the required courses, examinations and interviews. He will deliver his first public GPU training "Fundamentals of Accelerated Computing with CUDA C/C++" on April 21 and 22 online via Zoom. Further information and the registration form are available at indico.scc.kit.edu/event/2698/.

Security Problem with "TensorBoard" Application

TensorBoard is a visualization toolkit for the *TensorFlow* open-source machine learning platform. As such, it is quite popular with NHR@FAU customers who use TensorFlow regularly on our systems. However, we would like to raise your awareness of a security issue: On a multi-user system (such as the frontends of all NHR@FAU clusters), TensorBoard does not provide any access control; specifically, it opens a TCP/IP port that allows *anyone* with access to the node to execute any command on behalf of the TensorBoard user. An attacker could thus access private data, change and delete files, open further network connections, or execute malicious code. Unfortunately, the developers of TensorBoard are not inclined to provide a more secure access mechanism any time soon. Due to the huge security concern, we cannot recommend the use of TensorBoard on the cluster frontends for the time being. A possible workaround is to run TensorBoard on your local machine and "mount" the relevant NHR@FAU home directory via `sshfs`. For a detailed description, see: hpc.fau.de/?p=7968/#sshfs

New Specialist for Quantum Physics Simulations at NHR@FAU

On April 1, Dr. Florian Lange joined the NHR@FAU team of domain specialists. In 2019, Florian obtained his PhD in theoretical physics at the Chair for Complex Quantum Systems of the University of Greifswald with Prof. Holger Fehske. His expertise lies at the boundary of quantum physics and simulation, with a focus on low-dimensional condensed matter systems and tensor network algorithms. Florian is looking forward to work with customers from quantum physics and related fields to support them in their computing projects.

Full LIKWID Support in the Julia Language

We are happy to announce that the Julia wrapper `LIKWID.jl` now supports all features of the LIKWID library, including the MarkerAPI and full control over performance monitoring capabilities of CPUs and Nvidia GPUs. In addition, "management tasks" such as system topology queries and CPU frequency manipulation can now be performed from within Julia applications. The work on `LIKWID.jl` was started by Valentin Churavy (MIT Julia Lab) and continued by Carsten Bauer (PC^2 Paderborn). Find more details at hpc.fau.de/?p=11371.

Spotlight: Prof. Dr. Petra Imhof

Petra Imhof holds a professorship for computational chemistry and is the technical director of the Computer Chemistry Center at FAU. Her group's research deals with understanding (bio-)chemical and biophysical processes on an atomic level by molecular simulations. Of particular interest are protein-DNA interactions and enzymatic catalysis. Petra Imhof started her research career in laser spectroscopy, combined with molecular simulations (Ph.D. in 2001, University of Düsseldorf). After two postdoc positions, heading a junior group in Heidelberg, a professorship at the Physics department of the Freie Universität Berlin, and working as a professor for chemistry in Stavanger, Norway, Petra Imhof joined the FAU in 2020. At NHR@FAU, she is a principal investigator with a scientific focus on atomistic simulations. She also coordinates local activities in the Atomistic Simulation Center and in the NHR graduate school.

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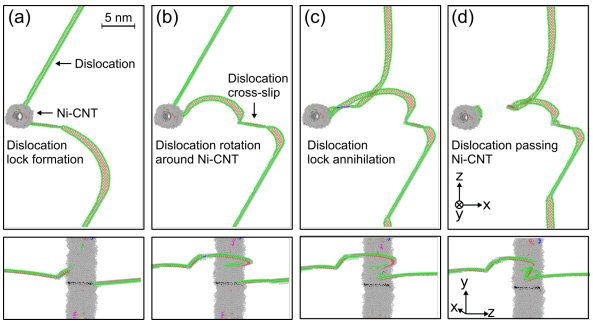
April Highlight: Dislocation-CNT Interactions in Al at the Atomic Level

Dislocation motion is the basic feature of plastic deformation of ductile metals. Anything that interferes with dislocation motion, such as grain boundaries, precipitates, or reinforcement particles, impedes dislocation slip and increases a metal's strength. Using molecular dynamics simulation, researchers from the chair of materials simulation (WW8) studied the interaction of pristine or Ni-coated carbon nanotubes (CNT) with lattice dislocations moving under stress in aluminum. It was shown that the embedded CNTs increase the stress needed to move dislocations (the yield stress) in a manner that is similar to an array of non-shearable precipitates that are by-passed via the so-called Orowan mechanism. However, the strain hardening mechanism associated with multiple dislocations intersecting CNTs on the same slip-plane was found to differ from the classical picture of Orwan hardening. The strengthening mechanisms observed in these simulations are much more complex and involve crystallographic and non-crystallographic cross-slip of near-screw segments on the CNT-metal interface, dislocation lock formation and annihilation, jog formation, and shedding of prismatic dislocation loops.



Snapshots from the third encounter of dislocation with a Ni-CNT. Red atoms represent the SF area. Green lines indicate partial dislocations. CNT and unstructured Al and Ni atoms around it are shown in gray color.

The large-scale atomistic simulations used to establish these complex mechanisms used the compute resources provided by the high-performance computing center at FAU Erlangen-Nürnberg (NHR@FAU). To learn more about the topic, see the paper by Samaneh Nasiri and Michael Zaiser at: doi.org/10.1016/j.mtla.2022.101347.