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## Quick News

### *Julia interface for LIKWID*

The University of Paderborn, the MIT Julia Lab, and NHR@FAU have worked together to provide a [Julia interface for LIKWID](#), specifically for using performance counters. You can now embed your Julia code with LIKWID markers!

### *Names for first NHR@FAU clusters*

In honor of FAU's [founders and early supporters](#), the first NHR@FAU clusters will be called *fritz* and *alex*, respectively. As reported in the June newsletter, MEGWARE will deliver and install the systems in late 2021.

### *RRZE looking for a new technical director*

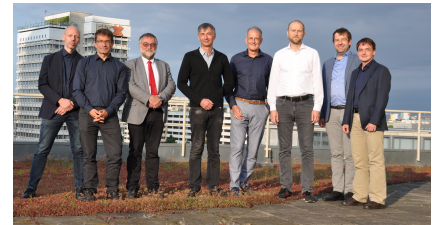
FAU has published a [job posting](#) for the position of technical director at Erlangen Regional Computing Center (RRZE). The application deadline is on October 17.

### *Missed a talk?*

The NHR@FAU YouTube channel at [tiny.cc/YT-NHR-FAU](https://tiny.cc/YT-NHR-FAU) provides recordings of some talks, lectures, and courses, as far as this is covered by copyright restrictions.

## NHR Association Officially Founded on August 23

In the presence of the representatives of the eight founding members, the *Verein für Nationales Hochleistungsrechnen – NHR-Verein* was founded in Berlin on August 23, 2021, with the signing of the bylaws. Prof. Christof Schütte (Zuse-Institut Berlin) was elected chairman of the board, which also comprises Prof. Gerhard Wellein (NHR@FAU)



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and Prof. Christian Pleschl (University of Paderborn). The chairman of the strategy committee, Prof. Rolf Krause, offered his congratulations: “With the founding of the association, the NHR-Verbund has taken the first step towards a nationwide coordinated infrastructure in high-performance computing. It is impressive to witness how quickly the NHR project has picked up speed, and how the eight centers are growing together already at this early stage.” The establishment of the association creates the institutional and scientific framework to jointly implement the goals of the NHR funding. You can read the [full GWK press release](#) (in German).

## Cx as a Service at NHR@FAU

NHR@FAU participates in the project *Cx as a service for sustainable HPC research software development* funded by the NHR committee. The goal is to provide resources for continuous testing in HPC software development projects. In collaboration with the Faculty of Physics at the University of Regensburg and the Chair for System Simulation at FAU, a system was created to build and run code on the [NHR@FAU Testcluster](#), which comprises a wide variety of architectures. These systems can be employed for Cx workflows using the [Gitlab instances at RRZE](#). The user can select specific nodes for their Cx jobs to build and run applications automatically. Test artifacts can be sent back to the Gitlab Cx system or to custom databases for further processing and evaluation. Besides *continuous integration*, i.e., build and coverage tests, the runtime data can be used for *continuous benchmarking* to track the performance of software changes. The Cx system is managed by NHR@FAU, and access is available on request. Details can be found in the [user documentation](#).

## Performance Engineering Tutorials Ahead

Our long-standing *Node-Level Performance Engineering* tutorial was accepted for the tenth time in a row as a full-day event at [SC21](#), the International Conference for High Performance Computing, Networking, Storage, and Analysis. SC21 is a hybrid event, with a mixture of face-to-face and online presentations. Georg Hager, Jan Eitzinger, and Gerhard Wellein will prepare video recordings of their tutorial and will be available for Q&A during the sessions. →

An extended version of the tutorial including hands-on exercises is offered as an online [PRACE training center event](#) on December 1–3, 2021. See the [registration page](#) for details.

## Spotlight: Dr. Jan Eitzinger

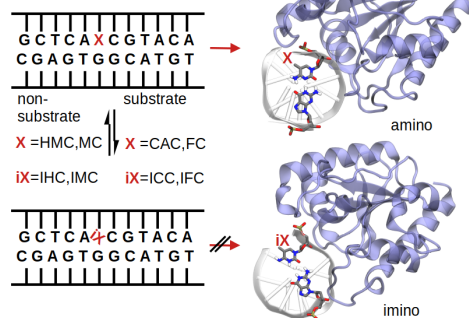


Jan Eitzinger heads the Software & Tools group of NHR@FAU since the beginning of 2021. Recent work covers the design and implementation of the *ClusterCockpit* performance monitoring stack, *The Bandwidth Benchmark*, the molecular dynamics performance toolbox *MD-Bench*, and the proposition of a markdown-based *performance logbook*. Besides development, he is involved in conducting performance engineering (PE) tutorials. Jan created the LIKWID Tools, had the initial idea for our successful ECM performance model, and proposed a bottleneck-centric PE process that is still a cornerstone of our PE efforts.

Jan's background is in chemical engineering, where he developed lattice Boltzmann methods during his master thesis at Prof. Durst's chair of fluid mechanics. He did his PhD at the systems simulation chair of Prof. Rde in the area of hardware-aware implementation of multigrid linear equation solvers. After two years working as a software developer in industry he joined the RRZE HPC group in 2009. Since 2019 he is a post-doc within the research group of Prof. Wellein at the FAU Computer Science department.

## October Highlight: Computing Alchemical Free Energies for a DNA-Processing Enzyme

The genomic information stored in the DNA can be distorted by, e.g., base damage or aberrant methylation. There are several DNA-processing enzymes that detect and repair such distortions. Thymine DNA Glycosylase (TDG) recognises and removes mispaired thymine and some forms of oxidized 5-methyl-cytosine. Recognition and discrimination of incorrect bases might occur



at several stages of the repair process: at TDG-DNA complex formation, when the base flips out of the DNA helix and into the enzyme's active site, or when the erroneous base is cut from the DNA. We conducted extensive molecular dynamics simulations of the DNA with different forms of oxidized 5-methyl-cytosine in free form and complexed to TDG at the local HPC clusters of RRZE. The atomic details of these simulations offer insights into the three-dimensional conformation of the DNA, the TDG enzyme, and how they interact in the complex. By applying a method called "thermodynamic integration," we can show that binding of the TDG enzyme to the imino forms of 5-methyl-cytosine is much more unlikely than binding of the corresponding amino forms. Surprisingly, the TDG-DNA complexes in the amino forms of 5-methyl-cytosine do not differ enough for substrate recognition by TDG, which therefore takes place at a later stage than TDG-DNA complex formation. Read the full story by Petra Imhof and coworkers at [DOI:10.3390/molecules26195728](https://doi.org/10.3390/molecules26195728)

## FAQ Corner: Cx

*Continuous Integration (CI)* is the practice of automatically integrating code changes into a software project. It relies on a code repository that supports automated building and testing. Often, CI also involves setting up a build system from scratch, including all dependencies.

*Continuous Testing (CT)* is the practice of executing automated tests as an integral part of the software development process. It tries to make sure that no functionality is lost and no errors are introduced during development.

*Continuous Benchmarking (CB)* can be seen as a variant of CT, where not only functionality but also performance is tested in order to avoid *regressions*, i.e., unwanted performance degradation due to code changes.

*Continuous Deployment (CD)* is the automatic deployment of the software coming out of the other Cx processes. This can be the installation on a particular system, rolling out a revision within a whole organization, pushing installation packages to public repositories, etc.

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