NHR@FAU Boosts Your Atomistic Simulations

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The Erlangen National High-Performance Computing Center (NHR@FAU) at FAU Erlangen-Nürnberg [1] was established in 2021 as a national center for HPC at German universities. Together with eight other institutions, it forms the NHR-Alliance [2]. NHR@FAU operates large-scale HPC systems and provides HPC services, related user support, and HPC training to members of German universities.

A strong focus of NHR@FAU lies on atomistic simulations and it also provides tailored hardware solutions in this area. As a key component of the NHR program, it offers exceptional competence and conducts extensive research in the field of atomistic simulations of molecular structures, with broad applications in chemistry, life sciences, materials science, and physics. With bundled atomistic structure simulation expertise, NHR@FAU helps users to select and use atomistic simulation methods in an HPC environment and actively accompanies and coordinates the development of high-performance simulation codes. An interdisciplinary approach promises not only synergy effects, e.g., through the exchange and joint development of simulation and evaluation tools, but in particular a cross-fertilization of materials and life sciences, which often use the same or similar simulation techniques.

The HPC research activities at NHR@FAU focus on performance engineering and modelling, performance tools, and research software engineering. NHR@FAU investigates and further develops hardware-efficient building blocks, programming concepts, and numerical algorithms for scalable, efficient, and robust iterative sparse matrix applications and stencil-based solvers on large-scale HPC systems.

A further core project is the education and lifelong training of scientists and engineers. The close cooperation among theory, simulation, and experiment, which has a long tradition in Erlangen, ensures that the training is not aimed specifically at modelers, but also made available to experimental colleagues. This is of particular importance in the light of increasing digitalization in science. NHR@FAU makes an essential contribution to the key technologies of scientific computing and scientific software development through the sustained concentration of methodological competence in both the application and development of computer codes and their hardware-related optimization.
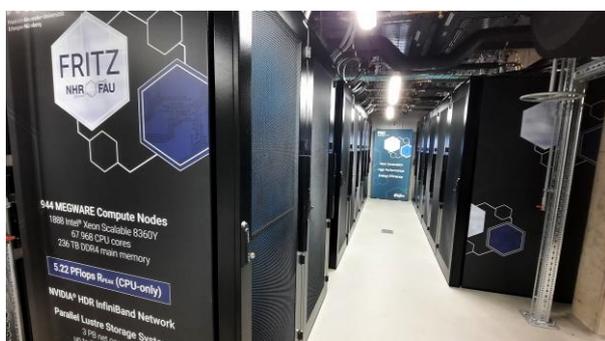
NHR@FAU main compute clusters:

← Fritz (CPU)

Alex (GPU) →

References
[1] https://hpc.fau.de
[2] https://www.nhr-verein.de/en