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ScalaLife - Improving the efficiency and scalability of Life Science Software - Talk by Erwin Laure

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Advances in HPC have transformed computational Life Science into an indispensable tool for both theoretical and experimental research. Peta- and upcoming exa-scale systems offer great possibilities for simulations and data processing. As usual software development is playing catch-up to hardware advances, even more so in the Life Science domain where computer engineering expertise is lagging relative to other fields. The ScalaLife project focuses on improving the scalability and efficiency of Life Science software and spreading the best practices among the community.
The project began work with four codes for molecular simulations –DALTON and ERGO (quantum mechanics), GROMACS (molecular dynamics) and DISCRETE (discrete molecular dynamics), thus covering a wide range of time-scales of physical processes. In this talk we will present the experiences gained by working with these packages and the results will also be reported in two PRACE white papers.

Erwin Laure is Guest Professor in Computer Science and Director of PDC-HPC, the High Performance Computing Center at the Royal Institute of Technology (KTH) in Stockholm, Sweden. Prior to this position he was the Technical Director of the EGEE project and now coordinates the ScalaLife project, aimed at improving the scalability of Life Science applications. Erwin holds a PhD in Business Administration and Computer Science from the University of Vienna, Austria. His research interests include grid and cloud computing with a focus on data management in grid environments as well as programming environments, languages, compilers and runtime systems for parallel and distributed computing, particularly exascale computing.

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