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Fostering interdisciplinary research by composable Julia software

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Today's ubiquitous data-driven workflows allow scientists to expand the limits of length and time scales in simulations. In my own field, namely first-principles atomistic simulations, the data itself is generated by systematic high-throughput workflows, which occupy a noteworthy chunk of the world's supercomputing resources. Questions related to the efficiency, robustness and accuracy of simulation protocols and the reproducibility of obtained simulation data are thus more pressing then ever. Due to the complexity of underlying physical models (non-linear PDEs, multi-linear algebra) tackling these issues is inherently an interdisciplinary endeavour. However, close collaboration of application scientists with researchers from mathematics or computer science requires software, which can support research thrusts all the way from model problems to full-scale applications.

I will discuss the opportunities of Julia programming language to satisfy the needs of interdisciplinary research. As an example I will focus on the density-functional toolkit (DFTK, https://dftk.org), a first-principle simulation code we started about 3 years ago. Being written entirely in Julia the code is highly accessible (only 7000 lines of code). At the same time Julia's composable programming paradigm allows (a) a seamless integration with standard HPC libraries (MPI, CUDA) and (b) to take advantage of unique features such as algorithmic differentiation. This has already enabled cross-disciplinary advances on error estimation or the developments of more robust algorithms. Notably, a number of these works involved undergraduates or PhD students from mathematics and computer science directly testing their work on relevant application simulations. Moreover the simplicity by which Julia enables code composability has stimulated joint initiatives to design common interfaces for sharing data within the young ecosystem. At the same time these efforts allow integrating with existing libraries outside Julia to avoid reinventing the wheel wherever possible.

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Sitzung Einordnung: Invited Talks