Large scale electronic structure simulations of complex magnetic objects

Daniel Wortmann, Institute for Advanced Simulation and Peter Grünberg Institut, Forschungszentrum Jülich, Germany

Complex magnetic structures are manifestations of the quantum-mechanical interactions in solids that are believed to form building blocks for future computing concepts like energy efficient data storage, neuromorphic computing, and possibly quantum computing. Currently, their theoretical description is mostly performed on a model basis which usually lacks a clear connection to the fundamental electronic properties of the underlying magnetic material. The standard model for such a description on the other hand is provided by density functional theory (DFT) and our well-established DFT code FLEUR (https://www.flapw.de) features much functionality tailored to describe complex magnetism.

Simulations using a DFT code like FLEUR for complex magnetic structures are extremely challenging due to the large system sizes needed and the difficulties in simulating all effects with sufficient accuracy due to the small energy scales involved. Hence, such calculations can only be performed on the supercomputers and we will report on our investigation performed on SuperMUC-NG within a GCS large scale project. In detail, we looked at the electronic structure of a Block point, a magnetic singularity in simpler magnetic models.

In addition to reporting on these DFT simulations of complex magnetic structures we will also discuss on the challenges faced and strategies employed when tuning a large legacy Fortran code for modern computing architectures. This includes the refactoring done to achieve good single-node performance using multithreading or GPU computing as well as the corresponding benchmarking. We will also discuss the scalability of the FLEUR code for different workloads and properties to simulate and the resulting future applicability.
The work has been supported by the MaX Center of Excellence in HPC (Horizon 2020 – 824143).