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A highly parallel KKR method and its applications in the study of magnetic defects of Fe-based alloys YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, G. MALCOLM STOCKS, AURELIAN RUSANU, Oak Ridge National Laboratory — Korringa-Kohn-Rostoker (KKR) method is a multiple scattering theory based all-electron ab-initio approach to the electronic structure calculations for solids. Its capability for calculating the Green function provides unique opportunities for us to study disordered alloys, defects, electronic transport, etc., from the first principles. In this presentation, we show the latest progress we made in parallelizing the KKR method. By exploring the computational parallization of the energy contour integration, k-space integration, and the scattering matrix inverse while keeping the scattering matrix data highly distributed, we are able to scale the KKR method to the thousands of processes (cores or processors). We also show a new way of performing parallel 3-D FFT that is used in our code for solving the electrostatic potential. Unlike conventional approaches to the parallel 3-D FFT, our method does not require global data transpose operations, which involve all-to-all communications between processes. We demonstrate the application of the KKR method for large scale applications in the study of magnetic defects in Fe-based alloys.

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