MIKA: A MULTIGRID-BASED PROGRAM PACKAGE FOR ELECTRONIC STRUCTURE CALCULATIONS

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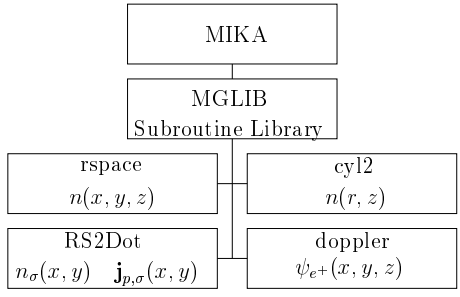
MIKA (Multigrid Instead of the K-spAce) [1] is a program package for quantum mechanical simulations of nanostructures [2, 3]. It consists of various applications, which solve the Kohn-Sham equations of density functional theory [4] (DFT) in different geometries (1D, 2D, axial symmetry, 3D). The equations are discretized on a real-space mesh, and solved using multigrid methods [5]. The central numerical techique in MIKA is the novel Rayleigh-quotient multigrid method [6] (RQMG).

In comparison to the more traditional plane-wave techiques, the real-space approach to electronic structure has the following advantages: flexible choice of boundary conditions, parallelization with domain decomposition, and availability of nonuniform grids. In addition, linear-scaling methods [7], where localized orbitals are needed, are most naturally formulated in real space.

We present an overview of the programs included in MIKA and give some examples of ongoing work related to the further development of the numerical methods and the software. We also present examples of research projects, where the MIKA-package is utilized.



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