UNIVERSITÄT SALZBURG

Fachbereich Mathematik
Hellbrunnerstraße 34
5020 Salzburg

Gastvortrag

Freitag, 21. Oktober 2016
15.30 Uhr
Seminarraum II

Dr. Kersten Schmidt
TU Berlin/TU Cottbus

High-order Mortar Finite Element Discretization for PDE Eigenvalue Problems in Quantum Chemistry

Abstract:

Mortar element methods use a decomposition of the computational domain and couple different discretization spaces in the subdomains weakly by a mortar condition. We use a high-order mortar element method for full-potential electronic structure calculations in Quantum Chemistry. For this we use a spherical discretization in spherical elements around each nucleus, which is adapted to resolve the core singularity due to an unbounded potential term. This spherical discretization is coupled to a finite element discretization in between the nuclei. We discuss the error of the mortar element method with uniform refinement as well as the reliability of a residual error estimator. With a series of numerical experiments we illustrate the theoretical convergence results for uniform refinement also in comparison with a conforming *hp*-adaptive finite element method and a *p*-adaptive refinement strategy based on the residual error estimator.

Einladender: Andreas Schröder