1 Workpackage 15

1.1 Mitarbeiter

An den Forschungsarbeiten in Workpackage 15 waren in diesem Jahr beteiligt:

- Univ.Prof.Dr.Karlheinz Schwarz
- Ao.Prof.Dr.Peter Blaha
- Dr.Robert Laskowski

1.2 Forschungsaktivitäten

The major computational tasks when solving the Kohn-Sham equations in solids is the numerical solution of a generalized eigenvalue problem. In a typical materials science problem we need to solve an eigenvalue problem of the order 1000x1000 to 50000x50000, but only 10-20 % of the lowest eigenvalues are needed.

The standard methods based on LAPACK or SCALAPACK libraries do not take advantage from the fact that we already have a solution of a very similar eigenvalue problem, namely that from the previous scf-cycle. One can take advantage of this knowledge in so called "iterative diagonalization" schemes. The methods best suited for this case are based on the Davidson-algorithm, but their efficiency depends a lot on a good "preconditioner", which needs to be efficient, but also needs to be evaluated quickly. We explored several possibilities and finally found a promising solution with a preconditioner that is based on the inverse of the Hamiltonian matrix. However, inversion of the matrix is not needed, but only a factorization of H enters the final equations.

This approach was implemented in an efficient (parallel) way and tested intensively for numerical accuracy and efficiency. It has a better scaling with the number of parallel processors than the standard SCALAPACK diagonalization routines. The importance of this development lies in the fact that we gained a speedup factor of about 10 for the diagonalization part, which now no longer is the dominant part of the calculations, while the setup of the matrix is even more costly than the diagonalization.

To illustrate the importance of this development we take a characteristic materials problem which could easily take a full year to solve on a single computer. Due to grid-computing (parallelization utilizing as many sites as possible) this can be reduced to one month, and due to the speedup of the new diagonalization the problem can finally be solved in two weeks.

It should also be mentioned, that such technical developments are very difficult to integrate and get funded in pure materials research projects, and thus the AGRID project provided a unique opportunity for us.

1.3 Publikationen

1.3.1 Publikationen in Journalen und Tagungsbänden

- R. Laskowski, P. Blaha, K. Schwarz: "Bonding of hexagonal BN to transition metal surfaces: An ab initio density-functional theory study"; Physical Review B, 78 (2008), 045409.
- H. Dill, J. Lobo-Checa, R. Laskowski, P. Blaha, S. Berner, J. Osterwalder, T. Greber: "Surface Trapping of Atoms and Molecules with Dipole Rings"; Science, 319 (2008), 1824.
- R. Laskowski, N. Christensen, P. Blaha, B. Palanivel: "Strong excitonic effects in CuAlO2 delafossite transparent conductive oxides"; Physical Review B, 79 (2009), 165209.
- R. Laskowski, T. Gallauner, P. Blaha, K. Schwarz: "Density functional theory simulations of B-K and N-K NEXAFS spectra of h-BN/transition metal(111) interfaces"; Journal of Physics: Condensed Matter, 21 (2009), 104210.
- P. Blaha, H. Hofstätter, O. Koch, R. Laskowski, K. Schwarz: "Iterative Diagonalization in APW Based Methods in Electronic Structure Calculations"; submitted for publication in Journal of Computational Physics.

1.3.2 Vorträge

- R. Laskowski: "h-BN on different transition metals, recent progres by ab-initio calculations"; Talk: Nanomesh - Final meeting of EU project, Orscholz, Germany; 06-22-2008 - 06-23-2008.
- K. Schwarz: "From crystal structure to materials properties with WIEN2k"; Keynote Lecture: International Symposium on Structure-Property Relationships in Solid State Materials, Nantes (invited); 06-29-2008 - 07-03-2008.
- R. Laskowski: "h-BN nanomesh on transition metal surfaces"; Keynote Lecture: CCP9 Conference 2008, Cambridge (invited); 09-04-2008 - 09-05-2008.
- K. Schwarz: "Electronic Structure of solids and surfaces: WIEN2k"; Keynote Lecture: International workshop on computational materials science, Cairo, Egypt (invited); 11-17-2008 - 11-20-2008.

- K. Schwarz: "How mathematics can speed up quantum mechanical calculations of solids"; Talk: 6th Vienna Conference on Mathematical Modelling MATHMOD 2009, Vienna (invited); 02-11-2009 - 02-13-2009; in: "Mathmod Vienna09", ARGESIM Reports, 34 (2009), ISBN: 978-3-901608-34-6; 386.

- P. Blaha: "Computational Materials Science with the WIEN2k code"; Talk: Computational Science and Engineering Workshop CSE2009, Rust; 01-08-2009 - 01-09-2009.

- K. Schwarz, P. Blaha, R. Laskowski: "A new iterative diagonalization for WIEN2k"; Talk: Projektkoordinierungstreffen AGRID-2, Linz; 04-28-2009.

- P. Blaha: "Magnetic and charge order phase transition in YBaFe2O5"; Talk: Psi-k meeting: "Magnetism in complex systems", Wien (invited); 04-16-2009 - 04-18-2009.

1.4 Lehraktivitäten

- *Vorlesung an der TU Wien: LVA 165.089: Physikalische und Theoretische Festkoerperchemie.* In dieser Vorlesung werden zuerst kurz die Grundlagen quantenmechanischer Berechnungen an Festkörpern besprochen, dann aber wird gezeigt, wie man mit unserem Programmpaket WIEN2k für einfache Kristalle Rechnungen durchführen kann. Zum Schluss wurden die Computeraspekte bis hin zu Grid Computing besprochen.