Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

A conventional, massively parallel eigensolver for electronic structure theory[1] V. BLUM, M. SCHEFFLER, Fritz Haber Institute, Berlin, Germany, R. JOHANNI, H. LEDERER, RZ Garching, TH. AUCKENTHALER, TH. HUCKLE, H.-J. BUNGARTZ, TU Munich, L. KRÄMER, P. WILLEMS, B. LANG, BU Wuppertal, V. HAVU, TKK Helsinki — We demonstrate a robust large-scale, massively parallel conventional eigensolver for first-principles theory of molecules and materials. Despite much research into $O(N)$ methods, standard approaches (Kohn-Sham or Hartree-Fock theory and excited-state formalisms) must still rely on conventional but robust $O(N^3)$ solvers for many system classes, most notably metals. Our eigensolver overcomes especially parallel scalability limitations, where standard implementations of certain steps (reduction to tridiagonal form, solution of reduced tridiagonal eigenproblem) can be a serious bottleneck already for a few hundred CPUs. We demonstrate scalable implementations of these and all other steps of the full generalized eigenvalue problem. Our largest example is a production run with 1046 Pt (heavy-metal) atoms [1] with converged all-electron accuracy in the numeric atom-centered orbital code FHI-aims,[2] but the implementation is generic and should easily be portable to other codes. [1] P. Havu *et al.*, Phys. Rev. B **82**, 161418 (2010). [2] V. Blum *et al.*, Comp. Phys. Comm. **180**, 2175 (2009).

[1]ELPA research consortium, funded by German Ministry of Research and Education (BMBF). http://elpa.rzg.mpg.de

Volker Blum
Fritz Haber Institute, Berlin, Germany

Date submitted: 24 Nov 2010 Electronic form version 1.4