Title

SCALABLE PARALLEL NUMERICAL METHODS AND SOFTWARE TOOLS FOR MATERIAL DESIGN

Authors

BYLASKA, EJ
KOHN, SR
BADEN, SB
et al.

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[G03.01] Scalable Parallel Numerical Methods and Software Tools for Material Design

E. Bylaska,S. Kohn,S. Baden,M.E.G. Ong,J. Weare (University of California, San Diego),A. Edelman (Massachusetts Institute of Technology),R. Kawai (University of Alabama at Birmingham)

A new numerical method of solution to the local spin density approximation is presented. The method is based on an efficient, parallel, adaptive multigrid eigenvalue solver. A preliminary test program is implimented using the LPARX parallel programming system which enables us to run the same code on a diversity of high performance parallel archetectures, including the CM-5, Paragon, Cray C-90, SP-1, and networks of workstations. It is shown that adaptivity is both necessary and sufficient to accurately solve the eigenvalue problem near the singularities at the atomic centers. While preliminary, these result suggest that direct real space methods may provide a much needed method for efficiently computing the electronic structures and forces on atoms in complex materials.

Part G of program listing