Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

VLab: A Collaborative Grid/Portal System for Computations of Materials Properties at High Pressures and Temperatures[1] PEDRO DA SILVEIRA, Minnesota Supercomputing Institute, University of Minnesota , CESAR R. S. DA SILVA, Minnesota Supercomputing Institute, University of Minnesota , RENATA M. WENTZCOVITCH, Minnesota Supercomputing Institute, Department od Chemical Engineering and Materials Science, University of Minnesota — We describe the development of a collaborative service-oriented architecture, the VLab, which handles from a single workflow the concurrent and distributed execution of multiple tasks involved in complex sequences of first principles calculations of materials properties at high pressures and temperatures. We demonstrate the usefulness of this system through a consolidated portal interface.

[1]Research supported by NSF/EAR and NSF/ITR programs

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Date submitted: 20 Nov 2006 Electronic form version 1.4