

Abstract Submitted  
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**VLab: A Service Oriented Architecture for Distributed First Principles Materials Computations**<sup>1</sup> CESAR DA SILVA, PEDRO DA SILVEIRA, RENATA WENTZCOVITCH, University of Minnesota, MARLON PIERCE, Indiana University, GORDON ERLEBACHER, Florida State University — We present an overview of VLab, a system developed to handle execution of extensive workflows generated by first principles computations of thermoelastic properties of minerals. The multiplicity ( $10^{2-3}$ ) of tasks derives from sampling of parameter space with variables such as pressure, temperature, strain, composition, etc. We review the algorithms of physical importance that define the system's requirements, its underlying service oriented architecture (SOA), and metadata. The system architecture emerges naturally. The SOA is a collection of web-services providing access to distributed computing nodes, workflow control, and monitoring services, and providing data analysis tools, visualization services, data bases, and authentication services. A usage view diagram is described. We also show snapshots taken from the actual operational procedure in VLab.

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