

Abstract Submitted
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Distributed Network-Based Verification and Validation of Electronic Structure Computations using ESTEST¹

GARY YUAN, Graduate Group in Applied Science, University of California Davis, Davis CA 95616, FRANCOIS GYGI, Department of Computer Science, University of California Davis, Davis CA 95616 — ESTEST is a web-based framework for verification and validation of electronic structure computations [1,2]. It enables automatic comparison and post-processing of simulation data obtained using Abinit, Quantum-Espresso, Siesta, Exciting, Qbox and VASP. We present new features of ESTEST that extend its operation to a distributed network of servers. This capability enables sharing, verification, validation, comparison, and post-processing of simulations across a decentralized network of ESTEST servers hosted by different institutions. Examples of cross-server operations including multiple servers will be demonstrated.

[1] G. Yuan and F. Gygi, Computational Science & Discovery 3, 015004 (2010) doi:10.1088/1749-4699/3/1/015004G

[2] <http://estest.ucdavis.edu>

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Francois Gygi
Dept of Computer Science, University of California Davis,
Davis CA 95616

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