

Abstract Submitted
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SC2IT: a cloud computing interface that makes computational science available to non-specialists¹ KEVIN JORISSEN, FERNANDO VILA, JOHN REHR, University of Washington — Computational work is a vital part of much scientific research. In materials science research in particular, theoretical models are usually needed to understand measurements. There is currently a double barrier that keeps a broad class of researchers from using state-of-the-art materials science (MS) codes: the software typically lacks user-friendliness, and the hardware requirements can demand a significant investment, e.g. the purchase of a Beowulf cluster. Scientific Cloud Computing (SCC) has the potential to breach this barrier and make computational science accessible to a wide class of non-specialists scientists. We present a platform, SC2IT, that enables seamless control of virtual compute clusters in the Amazon EC2 cloud and is designed to be embedded in user-friendly Java GUIs. Thus users can create powerful High-Performance Computing systems with preconfigured MS codes in the cloud with a single mouse click. We present applications of our SCC platform to the materials science codes FEFF9, WIEN2k, and MEEP-mpi. SC2IT and the paradigm described here are applicable to other fields of research beyond materials science, although the computational performance of Cloud Computing may vary with the characteristics of the calculations.

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