

Abstract Submitted  
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**High-performance scientific computing in the cloud**<sup>1</sup> KEVIN JORISSEN, FERNANDO VILA, JOHN REHR, University of Washington — Cloud computing has the potential to open up high-performance computational science to a much broader class of researchers, owing to its ability to provide on-demand, virtualized computational resources. However, before such approaches can become commonplace, user-friendly tools must be developed that hide the unfamiliar cloud environment and streamline the management of cloud resources for many scientific applications. We have recently shown that high-performance cloud computing is feasible for parallelized x-ray spectroscopy calculations.<sup>2</sup> We now present benchmark results for a wider selection of scientific applications focusing on electronic structure and spectroscopic simulation software in condensed matter physics. These applications are driven by an improved portable interface that can manage virtual clusters and run various applications in the cloud. We also describe a next generation of cluster tools, aimed at improved performance and a more robust cluster deployment.

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<sup>2</sup>J.J. Rehr et al., *CiSE*, **12**, 34 (2010)

Kevin Jorissen  
University of Washington

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