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Performance optimization of Qbox and WEST on Intel Knights Landing[1] HUIHUO ZHENG, CHRISTOPHER KNIGHT, Argonne National Laboratory, GIULIA GALLI, MARCO GOVONI, University of Chicago and Argonne National Laboratory, FRANCOIS GYGI, University of California Davis — We present the optimization of electronic structure codes Qbox and WEST targeting the Intel®Xeon Phi^{TM}processor, codenamed Knights Landing (KNL). Qbox is an ab-initio molecular dynamicscode based on plane wave density functional theory (DFT) and WEST is a post-DFT code for excited state calculations within many-body perturbation theory. Both Qbox and WEST employ highly scalable algorithms which enable accurate large-scale electronic structure calculations on leadership class supercomputer platforms beyond 100,000 cores, such as Mira and Theta at the Argonne Leadership Computing Facility. In this work, features of the KNL architecture (e.g. hierarchical memory) are explored to achieve higher performance in key algorithms of the Qbox and WEST codes and to develop a road-map for further development targeting next-generation computing architectures. In particular, the optimizations of the Qbox and WEST codes on the KNL platform will target efficientlarge-scale electronic structure calculations of nanostructured materials exhibiting complex structures and prediction of their electronic and thermal properties for use in solar and thermal energy conversion device.

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