Abstract Submitted
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Development and Use of Quantum Chemistry Methods on Intel Many-Integrated Core Units[1] EDOARDO APRA, Pacific Northwest National Laboratory — We will describe the approach we have taken in porting quantum chemistry algorithms based on local basis functions to the Intel MIC hardware. The implementation completed in the NWChem code shows the feasibility of effectively combining the processing power of traditional CPU architecture and coprocessor hardware on Petascale class computers. Benchmarks of scientific applications will be presented to illustrate the performances of large scale calculations.

[1]This work was conducted in the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), a national scientific user facility sponsored by DOE's Office of Biological and Environmental Research and located at PNNL

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