

Abstract Submitted  
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**OPAL: A New Multiscale Software Architecture Based on MPI-2** YUN-WEN CHEN, CHAO CAO, Quantum Theory Project and Department of Physics, University of Florida, MING ZHANG, Quantum Theory Project and Department of Computer and Information Science and Engineering, University of Florida, ERIK DEUMENS, Quantum Theory Project and Department of Chemistry and Department of Physics, University of Florida, HAI-PING CHENG, Quantum Theory Project and Department of Physics, University of Florida — Software integration for multi-scale simulations is a time-consuming process. Common practice is to turn the higher level calculation code ( e.g. DFT ) into a subroutine of the lower level calculation code ( e.g. MD ). This method often requires non-trivial effort. To avoid these difficulties, we have developed a software package OPAL, within which a minimal development effort is required to build a working multi-scale environment. We report our effort of integrating DL\_POLY and SIESTA codes for hybrid quantum-classical simulations. This work is supported the NSF through ITR-medium (NSF/DMR/ITR-0218957) program. The authors want to thank NERSC, CNMS/ORNL and the University of Florida High Performance Computing Center for providing computational resources and support that have contributed to the research results reported within this paper.

Hai-Ping Cheng  
Quantum Theory Project and Department of Physics, University of Florida

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