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Incoporating Existing Large Applications in the PUPIL System: Amber[1] SAM TRICKEY, QTP, Dept. Physics, U. Florida, JUAN TORRAS COSTA, U. Politecnica de Catalunya, GUSTAVO DE MIRANDA SEABRA, QTP, Dept. Chem., U. Florida, ADRIAN ROITBERG, QTP, Dept. Chem., U.Florida, E. DEUMENS, QTP and HPC Center, U. Florida — PUPIL (Program for User Package Interfacing and Linking)[1] inter-operates existing codes for multi-threaded, multi-scale quantum and classical mechanical simulations via JAVA, XML, JAVA, a C++ library, and minimally intrusive wrappers for each code. An architectural challenge for PUPIL is support of modules from a multi-scale QM-MD suite with much internal coupling. We have succeeded with the AMBER suite MD module (Sander), with Gaussian03 for QM. Our demonstration study is the decomposition of Angelis' salt with explict water. A variable quantum zone (solute and first solvation cell) was used, with the remaining waters via TIP3P. Sander calculated the Potential of Mean Force for the reaction through umbrella sampling, with the QM forces from Gaussian. We summarize PUPIL architecture and implementation aspects, report efficiency and overhead measures, and discuss the computed results.
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