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PUPIL: A New Concept of Software Integration in Multi-scale Simulations. JUAN TORRAS-COSTA, ERIK DEUMENS, SAMUEL TRICKEY, QTP, University of Florida — We present a relatively straightforward way to incorporate existing software packages systematically into a fully automated multi-scale simulation framework. The **PUPIL** (*Program for User Package Interfacing and Linking*) architectural concept is to provide a simulation manager, enabled by small, minimally intrusive wrapper routines installed within each software package. Thus prepared, the different packages ("Calculation Units") are plugged into the **PUPIL** system which one then operates as a software driver. A protocol is defined to communicate between the different Calculation Units and the **PUPIL** system to exchange information. The system has been designed using the OO paradigm and implemented in Java as a fast prototyping language. A test has been carried out joining three different packages to do a MD calculation with pattern recognition to identify the QM region and an external QM force calculation. The results show the ease of operation and maintenance of this software system with little overhead.
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