

Performance prediction for QuantumESPRESSO

P. Bonfà, F. Affinito, C. Cavazzoni

One of the goals of hardware software co-design is the evaluation of the effectiveness of different hardware solutions for the execution of the algorithms that constitute a given application used as reference. In this context, a performance model is an extremely useful tool that provides an estimate for the execution times and the data volumes of the main tasks of the application for a given set of hardware related parameters. In this presentation, the performance analysis conducted on the PW code of the QuantumESPRESSO suite and the subsequently obtained performance model will be discussed. Special attention will be devoted to the strategies adopted for the definition of the model and the problems encountered during the performance assessment. Finally, the accuracy provided by the current description and future perspectives will be reported.