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Simulations at the nanoscale on the Grid using Quantum ESPRESSO

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First-principle simulations based on density-functional theory have become quite common in the study of the matter at the nanoscale. Simulations for quite complex and realistic models are now within our reach, but such simulations are still considered HPC applications, requiring large vector or parallel computers with specialized hardware. In this talk I report on our experience on Grid utilization for realistic computations at the nanoscale, using the open-source Quantum ESPRESSO distribution of software.
The chosen application: calculation of phonon dispersions for a relatively complex crystal structure, is a prototype for simulations that are suitable for Grid computing, since it has moderate RAM requirements, long execution times, and it can be split into many semi-independent tasks. The Quantum ESPRESSO software, designed for execution on all kinds of machines from single PCs to massively parallel machines, was subject to minor modification to simplify the automatic splitting into many subtasks. A python interface takes care of scheduling tasks to the GRID, collecting results and re-scheduling failed tasks.
Our experience shows that in spite of the high failure rate, execution on the Grid compares favourably with MPI parallelization on conventional HPC hardware.

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