QUANTUM ESPRESSO: linear response codes on heterogeneous architectures

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As high-performance computing (HPC) approaches exascale, calculations that took hundreds of hours 30 years ago can now be performed in tens of seconds. For such class of machines, graphics processing unit (GPU) acceleration has become a *de facto* standard, and almost all of the first five entries in the Top500 list of supercomputers are heterogeneous architectures, based on GPU acceleration.

This context has proved to be particularly fertile for molecular and material sciences, that have evolved in parallel with the advances in computer science, and, nowadays, most of the main codes for molecular and material modelling have been ported or are in the process of being ported to heterogeneous HPC architectures.

In this respect, the QUANTUM ESPRESSO software suite **[1-4]** can boast a long experience, as the first accelerated working version of the `PWscf` code dates back to several years ago (2017) **[3]**. Since then, a big effort has been devoted to the improvement of the existing code and to the porting of new features to GPU-accelerated architectures.

With the new release (`qe-7.2`) almost all the main codes of the suite, including linear response codes, can be run on GPU, allowing to compute all the most relevant properties for spectroscopy and excited states (such as vibrational properties, EELS cross sections, optical absorption lineshapes) with a significant speed-up with respect to traditional architectures **[4]**.

In this presentation an overview of the state of the QUANTUM ESPRESSO software suite will be given, with particular emphasis on the recent porting of linear response codes on heterogeneous architectures **[4]**. Test cases on representative molecular systems will be presented, in order to provide a picture of results and performance that can be achieved and to discuss best practices that can be adopted in order to optimally run codes and exploit heterogeneous machines.

[1] Giannozzi P., et al., *J. Phys. Condens. Matter.*, 21, **2009**;
[2] Giannozzi P., et al., *J. Phys. Condens. Matter.*, 29, **2017**;
[3] Giannozzi P., et al., *J. Chem. Phys.*, 152, **2020;**
[4] Carnimeo I., et al., *J. Chem. Theory Comput.*, **2023** (accepted)