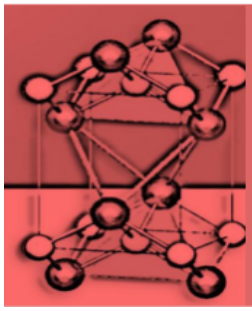

X Workshop on Novel Methods for Electronic Structure Calculations

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Trends in software for electronic structure calculations

Paolo Giannozzi [a]

[a] *DMIF Università di Udine and IOM-CNR, Italy.*

email:

First-principle calculations have become an exceedingly successful tool for the study of materials properties. Much attention is dedicated on the one hand to the application of old theories and the development of new ones; on the other hand, to the computed physical results. Less attention is paid to what stands in the middle, allowing to translate theory into materials properties: electronic-structure software.

In this talk I will provide my personal point of view on the state of the art and perspectives of electronic-structure software, notably in the framework of density-functional theory. I will briefly describe old and new problems in software development, posed by requirements of

- correctness and reproducibility,
- maintainability and interoperability,
- performance in both serial and parallel execution,
- portability on all kinds of hardware, and known solutions (or lack thereof).

Finally I will describe particular some recent improvements of the popular open-source Quantum ESPRESSO distribution, aiming towards "performance portability", that is: the ability to run with excellent performances on all modern computer architectures, in particular hybrid, GPU-accelerated ones that require extensive, architecture-dependent reorganization of codes. Performance portability is one of the main goals of the EU Horizon-2020 project MaX (Materials Design at the Exascale) whose main objective is to provide the community with high-quality, maintainable software that can be used for ambitious scientific goals on forthcoming "exascale" (capable of 10^{18} flops) machines.

[1]. "Quantum ESPRESSO: one further step towards the exascale",
I. Carnimeo, F. Affinito, S. Baroni, O. Baseggio, L. Bellentani, R. Bertossa, P. Davide Delugas, F. Ferrari Ruffino, S. Orlandini, F. Spiga, and P. Giannozzi,
Special Issue on "Software for Electronic Structure Based Simulations in Chemistry and Materials", J. Chem. Theory Comput. (2023), doi: 10.1021/acs.jctc.3c00249