The Abdus Salam International Centre for Theoretical Physics

Advanced Workshop on High-Performance & High-Throughput Materials Simulations using QUANTUM ESPRESSO

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Location : The Abdus Salam, International Centre for Theoretical Physics (ICTP)

The accuracy and predictive power of materials' simulations based on "first-principles calculations" allows nowadays to identify novel materials with improved or custom-designed properties and performance. The ever-increasing volume of computations and of data produced by them is triggering a scientific and technological revolution where behavior of ever-increasing complexity can be addressed in numerical experiments; where data and workflows' sharing can greatly enhance the synergies between different communities and efforts; and where services can be provided in the form of data, codes, expertise, workflows, turnkey solutions, and a liquid market of computational resources. Sustaining the effort that is supporting such a revolution will require a paradigm shift in software design and in the day-by-day work of materials simulation practitioners, based on the integration of concepts, tools, and applications from high-performance computing (HPC) on novel computer architectures and platforms and on high-throughput computing (HTC) on heterogeneous and geographically distributed computational resources. The challenge is here to run and manage an ever-increasing number of concurrent simulations (HTC) of ever-increasing size at an ever-increasing speed (HPC).

QUANTUM ESPRESSO (QE) has established itself as a leading open-source distribution of codes for quantum simulations of materials, with ~1000 paper/year (for usage analytics, see the link).

QE is based on density-functional theory, pseudo-potentials, and plane-wave basis sets. Besides being extremely flexible, versatile, and highly optimized on a broad variety of computer architectures, QE owns its popularity to a a very successful series of international training courses, run under the auspices of the Quantum ESPRESSO Foundation (QEF), often in collaboration with the Abdus Salam International Centre for Theoretical Physics (ICTP). Traditionally these schools address the fundamentals of quantum simulation of materials based on density-functional theory, occasionally with emphasis on some advanced applications (such as, e.g. computational spectroscopy, quantum transport, magnetism, etc.).

This *School* is the first specifically aimed at training simulation practitioners in the use of modern massively parallel HPC architectures (such as those currently available at the peta- scale level and foreseen to transition within few years to the exa- scale level) on one hand, and on the use of advanced tools for generating, managing, storing, and sharing results from HTC simulations, on the other. HTC training within the school being proposed will be based on the AiiDA infrastructure.

AiiDA (Automated Interactive Infrastructure and DAtabase for computational science) is a Python materials' informatics framework to manage, store, share, and disseminate the workload of high-throughput computational efforts, while providing an ecosystem for materials simulations where codes are automatically optimised on the relevant hardware platforms, and complex scientific workflows involving different codes and datasets can be seamlessly implemented and shared. Five active developers of the code are at EPFL (another main developer is at Bosch RTC in Cambridge, MA), and are complemented by two software engineers supported by the Swiss MARVEL project. AiiDA is designed around the four pillars of materials' informatics, as follows. At the low-level, AiiDA takes care of (1) automation and (2) data storage for the management and safeguarding of calculations, data and workflows. At the user-level, it provides an advanced and intuitive research (3) environment for accelerating scientific discoveries, and (4) sharing capabilities to enable collaborative research.