Materials Foundry: Development of High Performance Computing applications to leverage scientific discovery and technological advancement

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Materials are crucial to science and technology, to industrial competitiveness, and to face our major societal challenges: energy and environment, health care, information and communication, manufacturing, safety, and transportation. Against these needs, materials' simulations have emerged as one of the most powerful and widespread assets in the quest for novel materials (or "old" materials) with improved properties.

Materials modelling stands on the simulation of properties and processes at the molecular scale, which is performed thanks to powerful computer codes that operate as quantum engines of the simulation and that are extremely CPU- and energy-greedy. Present and future HPC systems, particularly those racing for exascale, are expected to be more and more heterogeneous (GPU-accelerated) in order to reduce power consumption, while enhancing the performance, and also enabling advanced data-oriented operations.

After a brief introduction and show-cases on materials modelling outcomes and impacts, I will present the activities of the spoke7/WP5 that is part of the new National Center High-Performance Computing, big data and quantum computing. In particular, the development of theoretical methods and HPC workflows for the predictive simulation of : i) traditional and advanced spectroscopies (support to experimental characterisation facilities), ii) (micro)structure and dynamics (catalysis, drug design), and iii) realistic time and length scale for industrial processes/devices.