Designing materials with HPC, a story of hardware, software, and theory

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Materials are crucial to science and technology and connected to major societal challenges ranging from energy and environment to information and communication, and manufacturing. Electronic structure methods have become key to materials simulations, allowing scientists to study and design new materials before running actual experiments.

This presentation aims at discussing how open-source community codes in electronic structure have evolved in order to enable the exploitation of frontier HPC for materials design and discovery. This had to take into account the development of HPC hardware (with a clear trend towards the deployment of GPU-accelerated machines), the software engineering required by the scientific community codes, and the emerging algorithms and electronic structure theoretical schemes that best fit this scenario.

Examples from the activities of the MaX (Materials design at the exascale) centre of excellence as well as from the ICSC centre (Centro Nazionale di Ricerca in High Performance Computing, Big Data & Quantum Computing) will be provided.