

Quantum ESPRESSO community code and the Exascale Challenge

Thursday, 25 February 2016 16:30 (25 minutes)

QUANTUM ESPRESSO builds upon electronic-structure codes that have been developed and tested by some of the original authors of novel electronic-structure algorithms and applied in the last twenty years by some of the leading materials modeling groups worldwide.

Innovation and efficiency are its main focus, with special attention paid to massively parallel architectures, and in the exascale challenge has been selected by many HPC centers, and technology providers world-wide as one of the application worth to be ported on new architecture. In the talk the refactoring effort and the porting strategies, toward exascale, will be presented and discussed together with preliminary results on new highly parallel chips.

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