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Advanced Workshop on High-Performance & High-Throughput Materials Simulations using Quantum ESPRESSO | (smr 3102)

Monday 16 January 2017

Day 1- Monday, January 16 - Adriatico Guest House - Kastler Lecture Hall Area (Lower Level 1) (08:30-18:30)

On-line video lectures recorded during the Workshop are available on the MaX (EU Centre of Excellence for Materials design at the Exascale) portal.

A Docker image was also create for this Workshop, including most of the material (script, input files, pseudopotentials, etc..) used for the lab-sessions.

!!! Link on overview page. !!!

time	title	presenter
08:30	Registration and Administrative Formalities	
09:30	DFT fundamentals: from theory to practice. Hohenberg-Kohn-Sham theory; variational principle; Hellman-Feynman th and energy derivatives.	S. BARONI
10:30	Coffee Break	
11:00	Implementation of DFT in QE: PPs, PWs, FFT, k-points.	R. GEBAUER
12:30	Lunch Break	
14:00	Docker Containers, Compiling and Running in a Container	R. INNOCENTE
16:00	Coffee Break	
16:30	DFT hands on: total energy scf calculations, optimizations, bands, dos, and post-processing; insulators vs metals (k-points); SCs: defects, isolated systems, surfaces.	P. GIANNOZZI PRESENTED BY IURII TIMROV