



Quantum ESPRESSO virtual hackathon 2021

Meeting's details

- Place:** Virtual meeting (using Zoom)
Link: <https://sissa-it.zoom.us/j/85813194629?pwd=Y2NiUWpINnl5bnNIU3NlOVlINmILdz09>
Meeting ID: 85813194629 **Password:** 456965
- Date & time (CET):** 15 January (14:00-18:00), 22 January (14:00-18:00), 29 January (14:00-18:00)
- Format:** Opening with an introductory brief talk (first and second day) or a brief summary from each group (second and third day); then work in breakout rooms in Zoom on the proposed topics (see list below).
- Objectives:** Update about the status of the Quantum ESPRESSO distribution; work on different topics to advance the development of the distribution; if possible, solve some of the open issues on Gitlab; decide the developments' plans for 2021.

List of participants

Name	Affiliation	15 Jan	22 Jan	29 Jan
Paolo Giannozzi	Uni Udine	+	+	+
Stefano Baroni	SISSA	+	+	+
Stefano de Gironcoli	SISSA	+	+	+
Pietro Delugas	SISSA	+	+	+
Iurii Timrov	EPFL	+	+	+
Oscar Baseggio	SISSA	+	+	+
Pietro Bonfà	Uni Parma	+	+	+
Fabio Affinito	CINECA	+	+	+
Daniele Cesarini	CINECA	+	+	+
Tommaso Gorni	ESPCI Paris	+	+	+
Matteo Cococcioni	Uni Pavia			+

Ivan Carnimeo	SISSA	+	+	+
Andrea Ferretti	CNR-NANO	+	+	+
Lorenzo Paulatto	IMPMC/CNRS/Sorbonne Université	+	+	+
Anton Kokalj	Jožef Stefan Institute	+	+	+
Andrea Urru	ETH-Zurich	+	+	+
Ye Luo	Argonne National Laboratory	+	+	+
Fabrizio Ferrari Ruffino	CNR-IOM	+	+	+
Flaviano José dos Santos	EPFL		+	+
Elena De Paoli	CNR-IOM	+	+	+
Jae-Mo Lihm	Seoul National University	+	+	+
Arles V. Gil Rebaza	Instituto de Física La Plata IFLP-CONICET	+	+	+
El-Abed Hadair	Sidney University	+	+	+
Akshaya Narayanasamy	IISER TVM		+	
Efracio Mamani Flores	UNJBG-PERU	+	+	+
Anoop A Nair	IISER TVM	+	+	+
Tobias Klöffel	RRZE-Friedrich-Alexander-Universität Erlangen-Nürnberg	+	+	+
Sagarmoy Mandal	Friedrich-Alexander-Universität Erlangen-Nürnberg	+	+	+
Hyungjun Lee	University of Texas Austin	+	+	+

Presentations

Introduction (January 15 th)	Paolo Giannozzi	Introduction and summary of main QE developments during 2020, plans for 2021
Profiling QE-GPU using Nsight tools (January 22 nd)	Filippo Spiga Louis Stuber	Starting from one or two input cases (which will be nice to crowdsource ahead of time), we showcase how to profile and understand bottlenecks in the code and (possibly) act accordingly.

		This is also an opportunity to learn about the tools and how to use them in an effective way.
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List of topics of the hackathon

Topic's name	Participants	Objectives
Merge of CPU and GPU distributions & GPU in linear-response codes	Paolo Giannozzi (coordinator) Pietro Bonfà Pietro Delugas Andrea Urru Stefano de Gironcoli Fabrizio Ferrari Ruffino Ivan Carnimeo Elena De Paoli Andrea Ferretti Fabio Affinito	<ol style="list-style-type: none"> 1.Fuse the q-e and q-e-gpu distributions into a single one 2.Implement OpenMP directives into the phonon code 3.Examine alternative ways to port to GPU
Miscellaneous	Lorenzo Paulatto (coordinator) Anton Kokalj Flaviano de Santos Pietro Delugas	<ol style="list-style-type: none"> 1.meta-GGA SCAN: improve stability; generalize the ATOMIC code to meta-GGA functionals 2.New interfaces and plugins 3.Fermi energy 4.APIs and documentation for FFTXlib & LAXlib 5.More suggested topics: <ol style="list-style-type: none"> a. improve EXX stability, especially with US/PAW b. improve robustness of symmetry detection c. tools to manipulate coordinates and cell, detect ibrav, rotate cell, build supercell, build a 2d cell
TDDFPT	Oscar Baseggio (coordinator) Tommaso Gorni Iurii Timrov Jae-Mo Lihm	<ol style="list-style-type: none"> 1.Porting of the magnon code into the develop version 2.Implement the pseudo-Hermitian algorithm in the magnon code 3.Add more documentation and clean-up the code 4.Implement the interface for solvers in LR_Modules

DFT+Hubbard	Iurii Timrov (coordinator) Paolo Giannozzi Matteo Cococcioni Akshaya Narayanasamy	<ol style="list-style-type: none">1. Redesign the input of the DFT+Hubbard2. Start the implementation of the multi-channel Hubbard manifolds3. Add more documentation; clean up the code.
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