

QUANTUM ESPRESSO

2020 Developers' Meeting at ICTP

Paolo Giannozzi, UniUd and IOM-CNR

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- *2019 good news:* the MaX CoE is in full activity ...
- *2019 bad news:* ... and now we have to deliver!

Deliver what exactly? “Porting QUANTUM ESPRESSO towards exascale!”

Planned actions

1. Extract from, and use in, MaX codes, portable
 - *libraries* (truly portable libraries!), and
 - *modules* (truly modular code!)
2. Extend MaX codes to hybrid architectures: GPU's, accelerators
 - a *portable* extension, that can be adapted to work with different hybrid architectures and maintained along with the current CPU code!
3. More conventional, but always valid, actions:
 - *improve algorithms:*
with better convergence properties, numerical stability, better optimized, better parallelized via reduced communications and bottlenecks
 - *improve the quality of the code:*
more readable, more re-usable, better documented, more tested, less buggy
 - *improve user documentation* (... an old problem!)

Suite of the meeting

- 10:00-10:15 Introduction (Paolo Giannozzi)
- 10:15-11:00 Optimization of CPMD and possible porting on QE (Tobias Kloeffel)
- 11:00-11:30 CMAKE for libraries and for QE (Daniele Cesarini)
- 11:30-12:00 Ongoing work on CP and PW alignment (Carlo Cavazzoni)
- 11:30-12:30 Round table discussion on:
 - state of GPU support (Pietro Bonfa', remotely)
 - devXlib (Andrea Ferretti, remotely)
- 14:00-14:30 New simplified GW code (Paolo Umari)
- 14:30 on Free discussion on future projects for
 - GPU's
 - LAXLib, FFTXLib, LRMods, PSLib libraries
 - any other subject of interest