

THEOS

THEORY AND SIMULATION
OF MATERIALS



ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

QE ADVANCED DEVELOPER TRAINING 2013



MOTIVATION

QE has been developed for *more than two decades* adding new features and capabilities over existing ones.

Today the distribution is composed of around *half a million code lines*, mostly written in FORTRAN 90, and it includes a number of different binaries.

Its complex structure can hinder further developments, especially by scientists not belonging to the small group of core developers.

To contrast this danger Paolo Umari proposed to organize some training activity specifically targeted to developers.

EVENTS IN 2013

Two Advanced Developer Training activities have been held in 2013

Quantum ESPRESSO Developer Training

(follow up of *Workshop on Computer Programming and Advanced Tools for Scientific Research Work*)

25 March 2013 - 28 March 2013 @ ICTP Trieste – ITALY

Organizers: P. Umari, P. Giannozzi, S. deGironcoli and I. Girotto

Advanced Quantum ESPRESSO Developer Training - QE HackFest :)

9 December 2013 - 19 December 2013 @ ICTP Trieste – ITALY

Organizers: E. Kucukbenli, S. deGironcoli, P. Giannozzi,
L. Martin-Samos and I. Girotto

QE DEV TRAINING

25 March 2013 - 28 March 2013 @ ICTP Trieste – ITALY

Organizers: P. Umari, P. Giannozzi, S. deGironcoli and I. Girotto

Objective: expand the knowledge in the community of the different aspects of development: methodologies and best practices. Learn how to best contribute to both the improvement and the maintenance of the package.

Around 37 participants from 18 different countries

4 organizers, 3 invited speakers (Cavazzoni, Dal Corso, Kucukbenli), and **30 attendees** (out of XX applications).

QE DEV TRAINING

25 March 2013 - 28 March 2013 @ ICTP Trieste – ITALY

Organizers: P. Umari, P. Giannozzi, S. deGironcoli and I. Girotto

4 full days of training:

The first three days morning lectures were followed by afternoon practical sessions addressing aspects such as:

- learning the most common components (Modules, variables, routines) of the QE package, including an overview of the parallel approach;
- learning how to perform standard tasks like wave-function I/O, calculating scalar product of 2 wave-functions, apply the Hamiltonian operator to a wave-function;
- learning how to develop a Post-Processing Tool based on existing QE components.

The last day was entirely devoted to advanced topics such as: LDA+U implementation and Atomic Wavefunctions, the Phonon package, the QE-GPU implementation and a vision in depth of the levels of parallelism, including a detailed introduction on how to perform large-scale simulation.

QE DEV TRAINING

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Organizers: P. Umari, P. Giannozzi, S. deGironcoli and I. Girotto

Feedback from the on-line evaluation:

Very positive appraisal of the relevance of the topics presented.
Less enthusiasm for the organization and presentation of the material.

Suggestions for future editions:

- more carefully prepared lectures;
- longer hands-on sessions;
- distribution of a written text with the supporting documentation;
- selection of a more homogeneous group of participants.

QEHACKFEST

9 December 2013 - 19 December 2013 @ ICTP Trieste – ITALY

Organizers: E. Kucukbenli, S. deGironcoli, P. Giannozzi,
L. Martin-Samos and I. Girotto

Objective:

Train a small group of next generation QE developers by a truly hands-on approach: implementing a real application (**Converse NMR approach**) into the current repository.

15 participants from 7 different countries
5 organizers, 1 invited speaker (A.P. Seitsonen), and
9 attendees (out of 65 applications).

- No ictp secretariat was assigned
- No computing resources was needed
- No fee, no subsistence
- Social occasions: dinner, take away pizza, birthday
- Single rooms at Adriatico, flexible hours

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Organizers: E. Kucukbenli, S. deGironcoli, P. Giannozzi,
L. Martin-Samos and I. Girotto

Previous feedback:

- more carefully prepared lectures;
- longer hands-on sessions;
- distribution of a written text with the supporting documentation;
- selection of a more homogeneous group of participants.

Addressed as

- Distribution of preparatory material on : *Intro to QE, SVN and QE-Forge, Intro to DFT, Intro to Fortran, Pseudopotential Theory, PAW Formalism, GIPAW* in three releases: Oct, Nov, Dec. With homeworks
- Two weeks of full immersion: theoretical and practical lectures intermixed .
- Carefull selection of a small group based on applicants' background and willingness to code. Ten (10) applicants were selected but one could not come for problems with university exams. Another participant had to leave earlier due to military duties.

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- Writing a post processing code – “sum_band” Brought up: Grids, Sizes
- Working in (shuffled) pairs
- Enough time for questions, discussions, and an encouraging environment
- Participants worked independently in constant presence of instructors
- Converse-NMR implementation (almost) from scratch:
 - Terms added to scf Hamiltonian
 - New initialization routines, new modules specific to converse-nmr
 - New routines to calculate orbital magnetization
 - Porting was more time consuming than writing from scratch, due to -no docs -unreadable code, mostly for the sake of little tricks/habits
- Testing, debugging in a workshop environment takes time but still useful.

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What worked

- Preparatory files, homeworks
- Number of participants, background, informal env., instructor presence
- Working in groups, Group presentations,
- Character of the added feature: not too invasive, not a pp either

What was suggested to be improved and how:

- More prep files, more questions, more time to digest
- Doing less (a new feature takes time to debug)
- More on challenges in group presentations
- ICTP being far from downtown
- A better location for social dinner than Scarpon

QEHACKFEST

“The 2 weeks that I spent in the training were more useful than any other conferences, workshops, etc. in my entire life. “

“Admittedly before the workshop I was quite doubtful about the formula "everyone learns from everyone". Eventually I had to change my mind. Indeed the workshop itself was structured in such a way to force collaborations among us.”

“It was always possible to ask them questions which they always answered serene without being patronizing/annoyed.”

“Getting a publication (hopefully!) out of the work we did will definitely be a plus!”

“Now that I know the most important internal operations in the Quantum Espresso, I would be really glad, if the ICTP can offer a further workshop to go even deeper and to extend the existing code by even more demanding routines.”

THANK YOU!