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**Hands-on Tutorial on Electronic Structure Computations**

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# Introduction to Quantum Espresso

P. Giannozzi
*Universita di Udine and IOM-Democritos*
*Trieste*
*Italy*

Strada Costiera, 11 - 34151 - Trieste - Italy • Tel. +39 0402240111 • Fax. +39 040224163 • sci_info@ictp.it • www.ictp.it
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# Introduction to QUANTUM ESPRESSO

*P. Giannozzi*
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# The QUANTUM ESPRESSO distribution

QUANTUM ESPRESSO: *Quantum opEn-Source Package for Research in Electronic Structure, Simulation, and Optimization*, is an integrated software suite for first-principle simulations, using density-functional theory (DFT), a plane waves (PW) basis set and pseudopotentials (PP)

QUANTUM ESPRESSO is the result of a IOM-DEMOCRITOS initiative, in collaboration with several other institutions (ICTP, CINECA Bologna, EPF Lausanne, Princeton University, Paris VI, IJS Ljubljana,...)

The main goals of QUANTUM ESPRESSO are

- *innovation* in methods and algorithms
- *efficiency* on modern computer architectures

A great effort is also devoted to *user friendliness* and to the formation of a *users' and developers' community*

# License

QUANTUM ESPRESSO is distributed under the *GNU (Gnu's Not Unix) General Public License (GPL)*, probably the most common free-software license (e.g.: the Linux Kernel). Basically:

- The source code is available.
- You can do whatever you want with the sources, but if you distribute any derived work, you have to distribute under the GPL the sources of the derived work.

Advantages:

- Everybody – including commercial entities – can contribute.
- Nobody can "steal" the code and give nothing back to the community.

# QUANTUM ESPRESSO as a distribution

QUANTUM ESPRESSO is a *distribution* of packages, rather than a single monolithic tightly integrated package. The core distribution contains the two main packages:

- `PWscf`: self-consistent electronic structure, structural optimization, molecular dynamics on the electronic ground state
- `CP`: variable-cell Car-Parrinello molecular dynamics

They share a common installation method, input format, PP format, data output format, large parts of the basic code. Also included:

- `PostProc`: graphical and postprocessing utilities (band structure, density of states, STM maps, ... )

# Packages

A set of packages, using routines from the core distribution, can be downloaded and installed on demand:

- `PWGui`: a Graphical User Interface for production of input files
- `PHonon`: linear-response calculations (phonons, dielectric properties)
- `NEB`: reaction pathways and barriers using Nudged Elastic Band
- `atomic`: atomic calculations, pseudopotential generation
- `PWcond`: ballistic conductance
- `XSpectra`: X-ray near-edge adsorption spectra (XANES) shifts
- `TDDFPT`: Time-Dependent Density-Functional Perturbation Theory

# More packages

Packages covering more advanced features, separately maintained but still requiring routines from the core distribution:

- `GIPAW`: Gauge-Independent PAW for EPR and NMR chemical shift
- `GWL`: GW band structure with ultralocalized Wannier functions

A package that adds functionalities to QUANTUM ESPRESSO by patching it:

- `PLUMED`: plugin for metadynamics calculations

# Plugins

Interoperable packages maintained by other groups that can be installed along with QUANTUM ESPRESSO and read its data file:

- `WanT`: Transport using maximally Localised Wannier functions
- `W90`: package for Maximally Localised Wannier functions
- `SaX`: electronic excitations from GW band structure
- `Yambo`: GW band structure, Bethe-Salpeter equations

# Organization

*Web site:* `http://www.quantum-espresso.org`

*Newsletter:* `pw_users@pwscf.org`, (sparingly) used by developers for announcements about QUANTUM ESPRESSO

*Mailing List:* `pw_forum@pwscf.org`, for general discussions
(all subscribed users can post)

*Developers' portal:* `QE-forge`, an integrated developer environment, open to external contributions in the field of atomistic simulations: `http://www.qe-forge.org`
The core distribution and packages is maintained in a single SVN tree. Available to everyone anytime via anonymous (read-only) access.

*Developers' Mailing List:* `q-e-developers@qe-forge.org`
(use this for technical questions or communications to developers)

# http://www.quantum-espresso.org

QUANTUMESPRESSO

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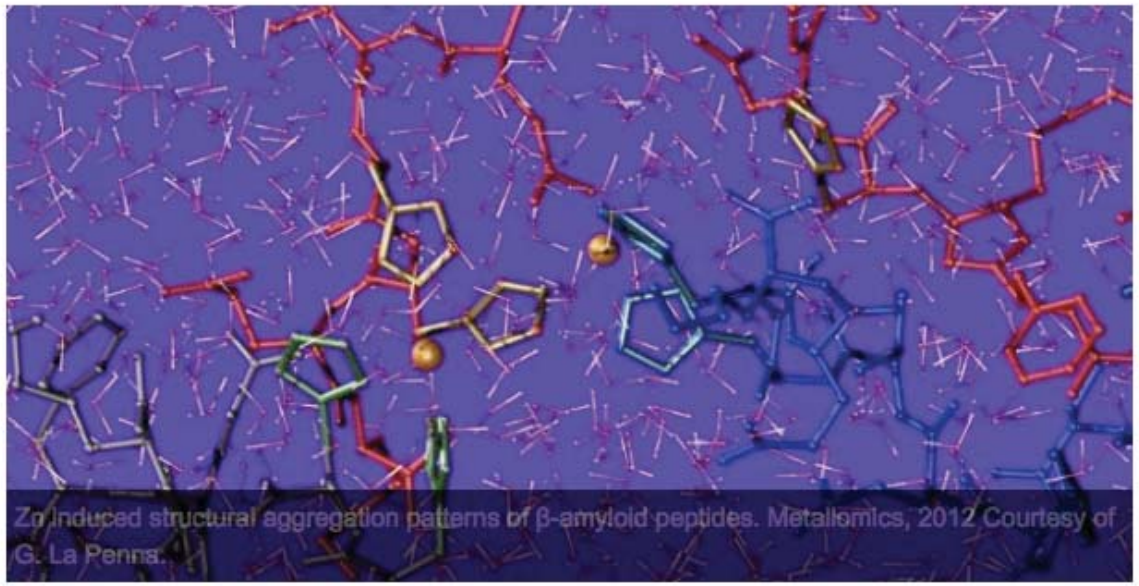
13.12.12

QUANTUM ESPRESSO EVENTS 2013

Hands-on Tutorial on Electronic Structure Computations, ICTP Trieste, 14-18 January.

Workshop on Computer Programming and Advanced Tools for Scientific Research Work & Quantum ESPRESSO Developer Training, ICTP Trieste, 11-28 March

(more events are planned, stay tuned)



Zn induced structural aggregation patterns of β-amyloid peptides. Metallomics, 2012 Courtesy of G. La Penna.

## QUANTUM ESPRESSO

is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.

# What can QUANTUM ESPRESSO do?

- Structural modeling (equilibrium structures of molecules, crystals, surfaces)
- Dynamical modeling (first-principles molecular dynamics) either on the electronic ground state (Born-Oppenheimer) or with fictitious electronic kinetic energy (Car-Parrinello)
- Chemical reactivity and transition-path sampling, using Nudged Elastic Band (NEB) method
- Linear response functions (vibrational and dielectric properties), plus some non-linear ones (third-order force constants and dielectric response, non-resonant Raman)
- Computational microscopy (STM)

# **Advanced** QUANTUM ESPRESSO **capabilities**

- Beyond simple DFT: DFT+U, nonlocal (vdW-DF), hybrid functionals (PBE0, B3LYP), meta-GGA
- Ballistic transport, transport with Wannier functions
- Free-energy sampling (metadynamics, with PLUMED plugin)
- Computational spectroscopy:
  - lattice and molecular vibrations: Raman, Infrared, Neutrons
  - magnons and spin excitations
  - photoemission (MBPT)
  - optical/UV absorption (TDDFT, MBPT soon to come)
  - NMR chemical shifts
  - X-ray spectra, core level shifts

# Using PWscf

The main executable of PWscf is `pw.x`. It reads data from an input file: e.g. `pw.x -inp` *input_file* having the following structure:

```
&NAMELIST1 ... /

 &NAMELIST2 ... /

 &NAMELIST3 ... /

 INPUT_CARD1
  ....
  ....
 INPUT_CARD2
  ....
  ....
```

NAMELISTS are a standard input construct in fortran90.

The use of NAMELISTS allows to specify the value of an input variable only when it is needed and to define default values for most variables that then need not be specified. Variable can be inserted in any order.

INPUT_CARDS are specific of ESPRESSO codes and are used to provide input data that are always needed and would be boring to specify with the `variable_name=variable_value` syntax used by NAMELIST.

INPUT_CARDS require data in specific order (which may depend on the situation and on the value of a card_format_specifier )

For instance:

```
INPUT_CARD   card_format_specifier
 data(1,1) data(1,2) data(1,3) ...
 data(2,1) data(2,2) data(2,3) ...
 data(3,1) data(3,2) data(3,3) ...
 ... ... ...
```

Logically independent INPUT_CARDS can be given in any order

# Namelists (1)

There are *three mandatory* NAMELISTS in PWscf:

| | |
|---|---|
| `&CONTROL` | `input variables that control the flux of the calculation and the amount of I/O on disk and on the screen.` |
| `&SYSTEM` | `input variables that specify the system under study.` |
| `&ELECTRONS` | `input variables that control the algorithms used to reach the self-consistent solution of KS equations for the electrons.` |

# Namelists (2)

Two additional NAMELISTS in PWscf *must* be specified under certain circumstances:

```
&IONS      needed when ATOMS MOVE! IGNORED otherwise !
           input variables that control ionic motion in
           molecular dynamics run or structural relaxation

&CELL      needed when CELL MOVES! IGNORED otherwise !
           input variables that control the cell-shape
           evolution in a variable-cell-shape MD or
           structural relaxation
```

# INPUT_CARDS (1)

There are *three mandatory* INPUT_CARDS in PWscf:

```
ATOMIC_SPECIES    name, mass and pseudopotential used for
                  each atomic species present in the system
ATOMIC_POSITIONS  type and coordinates of each atom in the
                  unit cell
K_POINTS          coordinates and weights of the k-points
                  used for BZ integration
```

and a few more that must be specified *only* in some cases:

```
CELL_PARAMETERS
OCCUPATIONS
CONSTRAINTS        (only for constrained dynamics)
```

**A sample (and simple) input file**

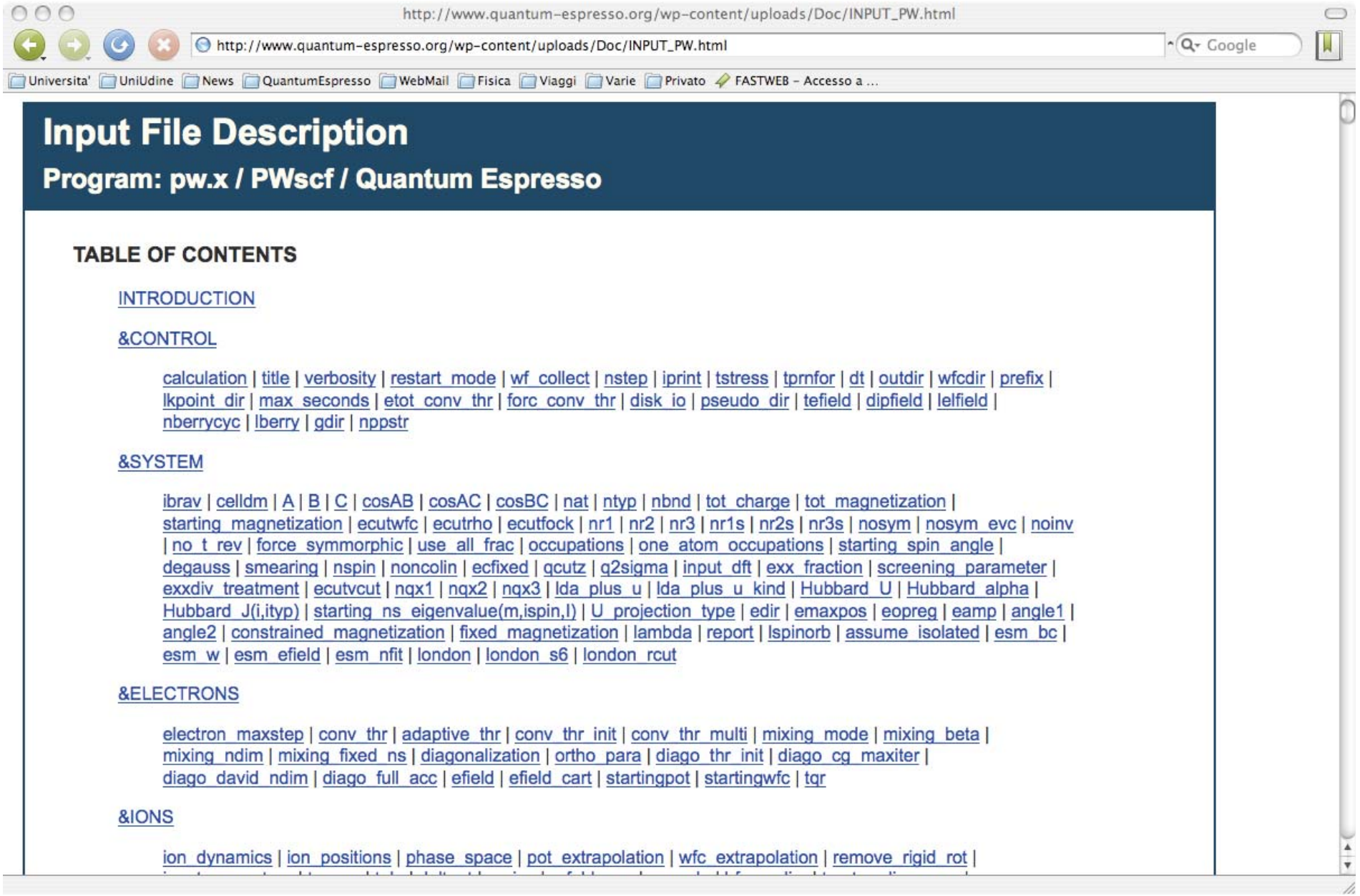
```
 &control
    calculation = 'scf',
    prefix = 'Si_work',
    tprnfor = .false.,
    pseudo_dir = '.',
    outdir = '.'
 /
 &system
    ibrav =  2,
    celldm(1) = 10.0,
    nat =  2,
    ntyp = 1,
    ecutwfc = 15,
    nspin = 1,
 /
 &electrons
    mixing_beta = 0.7
 /

ATOMIC_SPECIES
 Si 28.086  Si.pbe-rrkj.UPF

ATOMIC_POSITIONS (alat)
 Si 0.0 0.0 0.0
 Si 0.25 0.25 0.25

K_POINTS (automatic)
  3 3 3 1 1 1
```

# Online input documentation



# Location of files

Use environment variable `$WORKSHOP` to locate where the files are, but *please do not work there!* Copy needed files to your machine.

```
$WORKSHOP = /afs/ictp/public/shared/smr2522
```

Exercises for today are in `$WORKSHOP/day1`

Local copy of the documentation useful today is in

```
$WORKSHOP/espresso-5.0.2/PW/Doc/INPUT_PW.html
$WORKSHOP/espresso-5.0.2/PP/Doc/INPUT_BANDS.html
$WORKSHOP/espresso-5.0.2/PP/Doc/INPUT_DOS.html

$WORKSHOP/espresso-5.0.2/CP/Doc/INPUT_CP.html
```