



QE Developers meeting

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AiiDA - QE communications

- The main challenge is to facilitate as much as possible the interaction between different codes.
- Focus on **i/o**.
- Desideratum: serialize all relevant information in an XML file, to be “copied and pasted” inside a database.
- Note: easiest for machine does not coincide with easiest for humans!

XML usage example

This is the desired (python) code to read an XML and retrieve a dictionary to be stored in the database:

```
import xmldict
with open('data-file.xml') as f:

    parsed_dict=xmldict.parse(f.readlines())
```

The parsing is very simple, but the data usage is tricky!

This or other simple forms of XML parsing can works only if XML is written in a **standard** and **documented** way!

Current XML in QE

- **input:** XML input is a welcome addition, but not indispensable. AiiDA creates the usual text input, and if the input file is human-readable, it is easier for the user to double-check it

(From past experience in QE: *challenging* to keep the XML aligned with the text input!)

- **output:** the XML file can contain a lot of information, more accessible than the standard output (in principle!)

Pro: a well designed XML file does not need maintenance in the parsing. New elements stored in the XML can be automatically stored and read. On the contrary, a new information in the standard output requires a manual modification in the QE parser!

Challenge: must be automatically **readable** and **usable**

Some inconsistencies

<CELL>

```
<LATTICE_PARAMETER type="real" size="1" UNITS="Bohr">  
  3.026526E+001  
</LATTICE_PARAMETER>
```

Redundancy
with celldm(1)

<DIRECT_LATTICE_VECTORS>

```
<UNITS_FOR_DIRECT_LATTICE_VECTORS UNITS="Bohr"/>  
<a1 type="real" size="3" columns="3">  
  3.026526E+001  0.000000E+000  0.000000E+000  
</a1>
```

Tagname
changes

Different formats
for vectors

Different formats
for units

<IONS>

```
<ATOM.1 SPECIES="K  " INDEX="1" tau="4.025825E+000 3.832990E  
+000 4.013289E+000" if_pos="1 1 1"/>  
<ATOM.2 SPECIES="Nb " INDEX="2" tau="2.0214542E+000 6.123597E  
+000 1.196735E+000" if_pos="1 1 1"/>
```

- Some missing information, like the total energy...

XML group

Original tasks:

- Merging of the different routines used to write the XML file;
- Adding to the XML file the missing information;
- Design of a new XML schema.

XML group (2013)

In the XML branch of QE

- Merged the PW and CP reading and writing of the xml data-file.
- "qexml.f90" is now the only library used for XML management.

Thanks to Simone Ziraldo!

- **Need volunteers to test the restarts of PW and CP before merging into trunk!**

XML group (2014)

1. **Add more info in the XML file:**

- missing physical properties: total energy, forces, stresses, ...
- which algorithms are used;
- Data obtained by specific routines calls (Berry phase polarization, +U occupations, ...);
- All the informations coming from the input;
- trajectories for relax, vc-relax, MD (positions, cells, velocities, energies) in a separate **documented** file, if requested;
- log of warnings / errors in a parsable format;

2. Write the XML file in an **appropriate** format.