

PWscf + XCrySDen: **Advanced I/O handling**

(part-II)

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XCrySDen → **PWgui** → **PWscf**

Basic scheme ...

prepare by **PWgui**



pw.x < **stdin** > **stdout**



analyze by **XCrySDen**

- perform SCF calculation:

PWgui

pw.x < **stdin** > stdout

analyze by **XCrySDen**

output: *prefix.**

- calculate property:

PWgui

pp.x < **stdin** > stdout

output: *filplot*

- filter (transform) the data:

PWgui

chdens.x < **stdin** > stdout

output: *fileout*

analyze by **XCrySDen**


PWgui == PWscf GUI

- ✓ is free software (GNU General Public License)
- ✓ WEB page:
<http://www.pwscf.org/>, there is link to:
<http://www-k3.ijs.si/kokalj/pwgui/>

PWgui and GUIB project

CONSIDER: inputs for numerical simulation software are simple from computer perspective

IDEA: construct a two-purpose meta-language:

- define the input syntax
 - provide automatic GUI construction
- 

GUIB: simple **G**raphical **U**ser **I**nterface **B**uilder

<http://www-k3.ijs.si/kokalj/guiB/>

GUI based on GUIB

- a GUI based on GUIB closely follows the structure of the input
- example:

```

water molecule
&parameters
  job_type   = optimization
  functional = B3LYP
  basis_set  = 6-311G
&end
Input_Geometry
H   0.000   0.773  -0.555
O   0.000   0.000   0.139
H   0.000  -0.773  -0.555
End
  
```

The screenshot shows a window titled "Simulation Setup (No.0)" with a "File" menu. The interface is organized into sections:

- Line: Title**: A text input field for "Job title" with a "Help" button.
- Namelist: Parameters**: A table of parameters with dropdown menus and "Help" buttons.

Job type:	Structural optimization	Help
DFT Functional:	B3LYP	Help
Gaussian basis set:	6-311G	Help
- Enter atomic coordinates**: A section containing a table of atomic coordinates.

	Atomic symbol	X-Coordinate	Y-Coordinate	Z-Coordinate
1	H	0.000	0.773	-0.555
2	O	0.000	0.000	0.139
3	H	0.000	-0.773	-0.555

- the function of such GUI is to manage input files (creation + editing)

PWgui Installation

- **define PWGUI** environmental variable to point to package root-directory

- **add PWGUI** to the PATH

- **for csh-like shells (edit ~/.cshrc):**

```
setenv PWGUI /path/to/pwgui
```

```
set path = ( $PWGUI $path )
```

- **for Bourne-type shells (edit ~/.profile or ~/.bashrc):**

```
PWGUI=/path/to/pwgui; export PWGUI
```

```
PATH=$PWGUI:$PATH
```

- **now source the profile:**

```
for Csh: source ~/.cshrc; rehash
```

```
for Bash: . ~/.bashrc
```

- **execute: pwgui**

PWgui: what it provides?

- manage (create and edit) inputs for the following modules:

`pw.x`

`ph.x`

`pp.x`

`chdens.x`

`projwfc.x`

`d3.x`

- contain help:
 - User's manual
 - INPUT_* files
 - description of individual variables (**Help** buttons)
- visualization of structure: PWgui uses XCRYSDEN

PWgui: create a new pw.x input

- select menu: **File->New Input ...->New PW.X Input**
- **PWgui** opens a new page and this page holds several pages:
 - + one page per each namelist
 - + one page for CELL_PARAMETERS/ATOMIC_SPECIES/ATOMIC_POSITIONS cards
 - + one page for K_POINTS card
 - + one page for CLIMBING_IMAGES/OCCUPATIONS cards

PWgui: display help for pw.x

- description of variables:
use **Help** buttons on the right
- description of whole pw.x input:
select menu: **Help->PW.X Input Syntax**
- PWscf User's manual:
select menu: **Help->PWSCF User's guide**

PWgui: event driven mechanism

- on *Control* page select:
`Type of calculation = Self-Consistent-field`
- goto *Ions* page: all items are disabled
- on *Control* page select:
`Type of calculation = Ionic-relaxation`
- goto *Ions* page: some items are enabled now.
- select a given type of ionic dynamics (first item): more items get enabled ...

PWgui: editor vs. GUI mode

- execute:

```
cd $PWGUI  
pwgui
```

- select menu: **File->Open Input ...->Open PW.X Input**
- choose a given file from: **examples/pw/** directory (for example: **si.scf.in**)
- now try the following menu items:
 - **View->Input file**
 - **Edit->Input with editor**
 - **Edit->Input's copy with editor**

PWgui & XCRYSDEN: visualization

- try menu: **View->Structure with XCRYSDEN**
(XCRYSDEN will display structure)
- then select the **PWgui** menu: **File->Settings**
 - on ***PWgui settings*** page select:
 - **launch XCRYSDEN = in notebook page**
- retry the menu: **View->Structure with XCRYSDEN**
(XCRYSDEN will appear inside PWgui as a new notebook page)

PWgui: input error checking

- select menu: **Edit->Input with editor**
- do an error on purpose, for example, add an undefined variable:

```
&CONTROL
```

```
my_var = 'my_value',  
calculation = 'relax',  
...
```

- save the file and exit from editor: **PWgui will complain !!!**
- **Message:** when PWgui complains about input, then the input probably contains syntax errors !!!

PWgui: about modules

- modules are defined in `$PWGUI/modules` directory
- each module is in its own directory
- example: `pw.x` module:
 - located in `pw/` subdirectory
 - files:
 - » `pw.tcl` — definition of input syntax and GUI
 - » `pw-event.tcl` — event driven mechanism
 - » `pw-help.tcl` — help for variables
 - » `commands.tcl` — various functions for GUI

More info on Installation

- **PWgui** is written in [incr Tcl], which is a scripting language:
 - **ADVANTAGE:** no compilation
 - **DISADVATAGE:** requires [incr Tcl] and related software
- How to install [incr Tcl] and related software:
 - Compile sources:
 - For Tcl/Tk see: <http://www.scriptics.com/>
 - For ITcl/Itk/Iwidgets see: <http://incrtcl.sourceforge.net/>
 - Binaries (for a few platforms only)
 - ActiveTcl (contains everything): <http://aspn.activestate.com/ASPN/Tcl>
- Today we have used a self-contained package for Linux-x86 !!!

Do an example yourself

- Take, for example, the input files from the **PWscf** package (example-5):
 - **`pw_examples/example5/reference/`**
- You will need the following two files: **`si.scf.in,`**
`si.pp_rho.in`
- Edit the files using **PWgui** and modify correctly variables such as **`outdir,`** **`pseudo_dir,`** ...

Do an example yourself (cont.)

- Execute something like:
 - `pw.x < si.scf.in > si.scf.out`
 - `pp.x < si.pp_rho.in > si.pp_rho.out`
- Then create a `chdens.x` input file using PWgui.
- When done, do:
 - `chdens.x < my.file.in > my.file.out,`
 and visualize result with XCRYSDEN.