CRYSTAL_GUI installation instruction

by Piero Ugliengo

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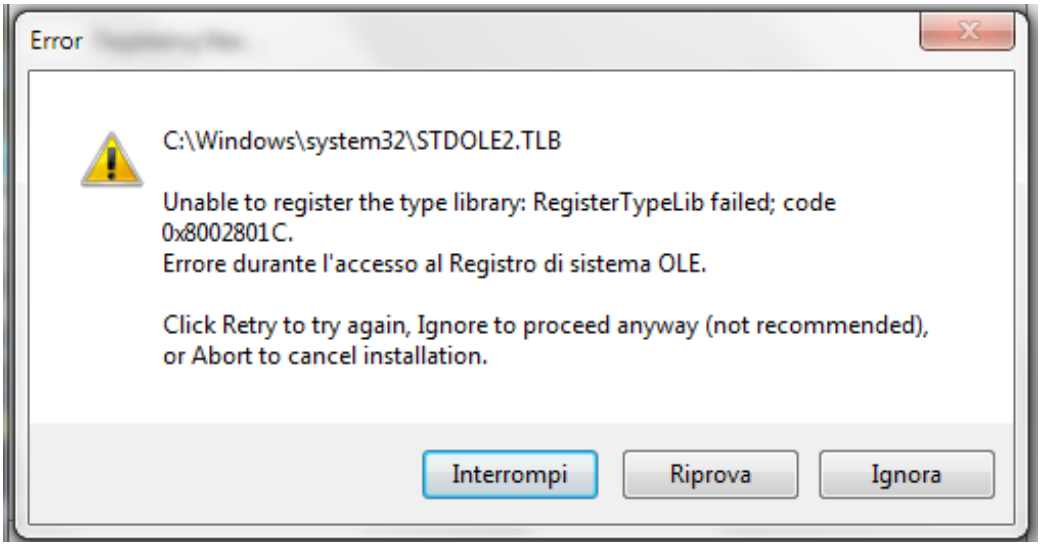
Copy the `crystal_gui_setup.exe` in a temporary directory. To install crystal_gui double-click it and then follows the usual steps. Please also read carefully the license agreement. At the end a new item crystal_gui is also added to the list of programs.
Under Windows Vista and Windows 7 a minor problem when registering some libraries arises with an error similar to this one:



Just select Ignore to finalize the installation. To put the crystal_gui icon on the desktop press the Start button and locate the 

item. Right-click on the icon and drag it to the desktop in order to create a link to the application.

To start crystal_gui double-click on the corresponding icon: 

CRYSTAL_GUI Help file

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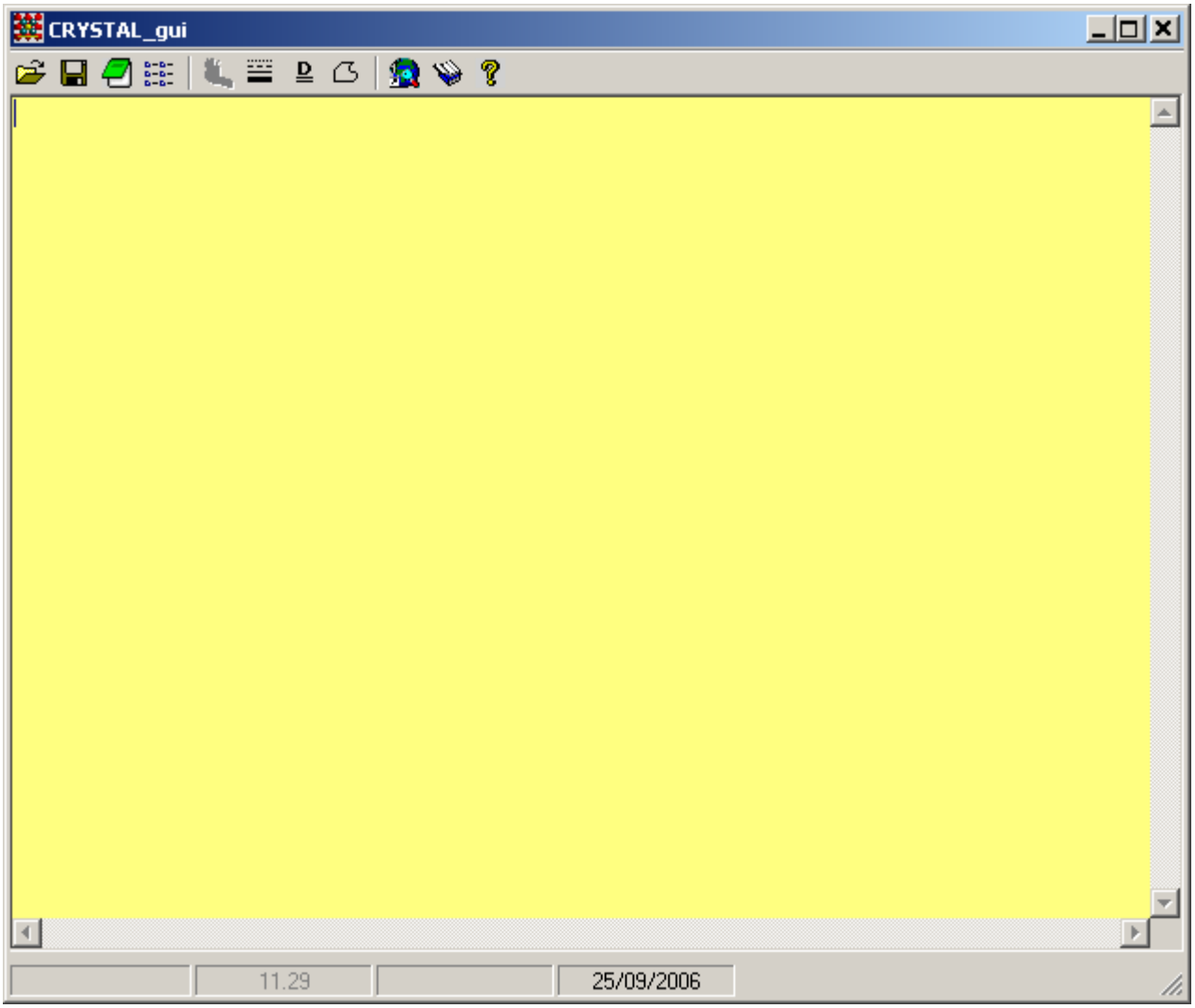
CRYSTAL_gui is a simple graphic user interface to CRYSTAL periodic quantum mechanical code (http://www.crystal.unito.it). It allows to run CRYSTAL and PROPERTIES within a window framework which wraps the input (.d12 or .d3 files) and the corresponding output files (.out files). It also allows to run programs to make maps of electronic charge or electrostatic potential, to plot density of states (DOS) and bands structure. If the user has also installed the Ghostscript/Gsview program it will automatically render the postscript files to the screen.

To start *CRYSTAL_gui* double-click on the corresponding icon:

A yellow background window pops up:



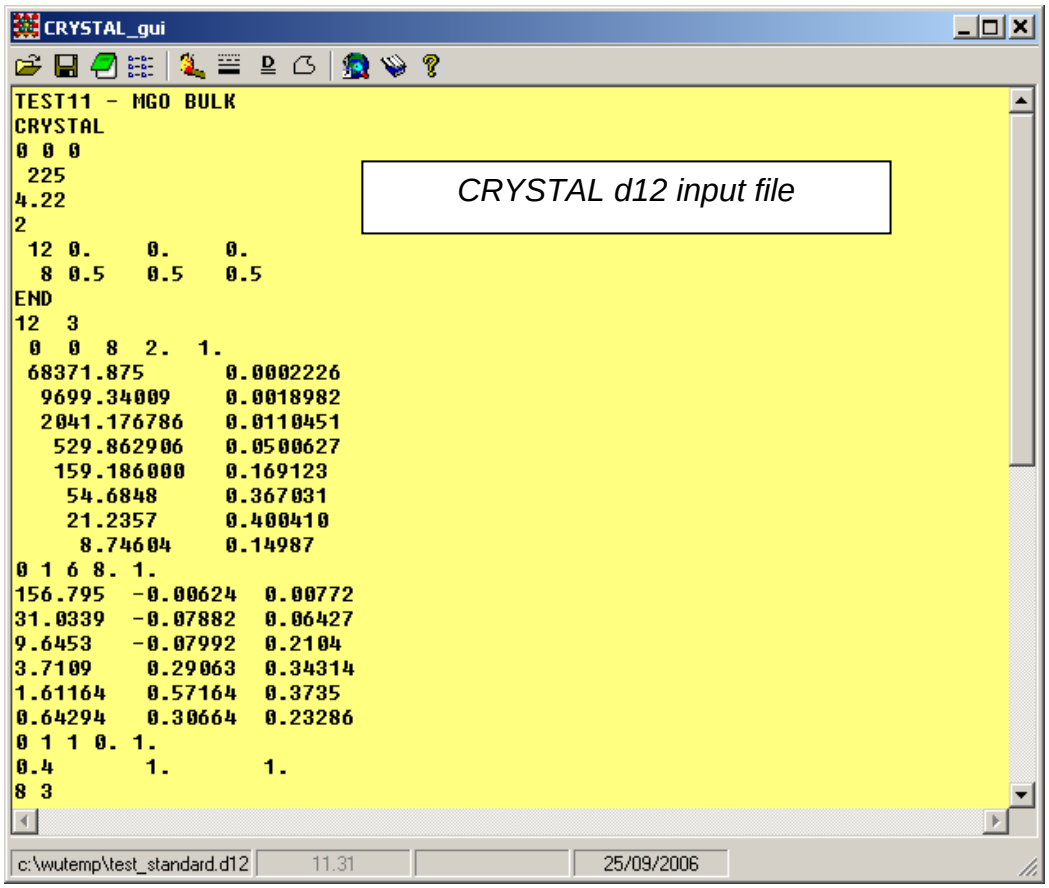
The icons in the toolbar allow to manage input files and to launch a variety of programs.

Their detailed meaning is reported in the following:

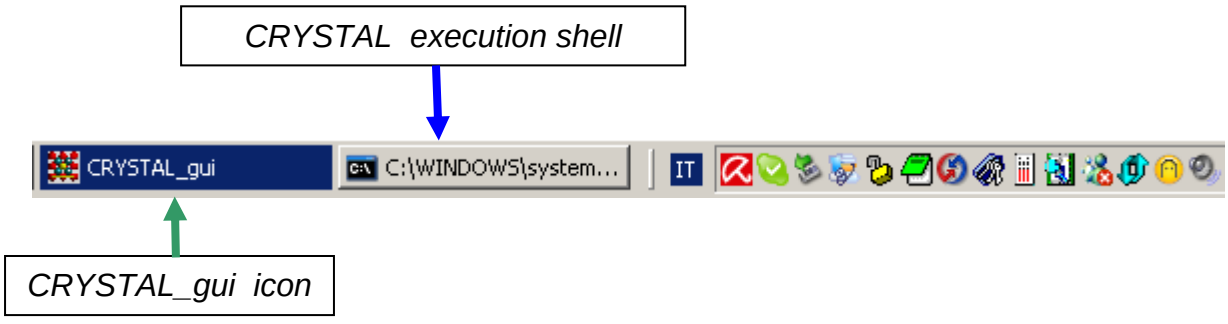
Open a .d12 or .d3 input file
Save a modified .d12 or .d3 input file
Edit the actual file using a user specific editor
Remove all fortran (fort.xx) files from the actual directory
Submit a CRYSTAL/PROPERTIES run using the current .d12/.d3 input file
Run BAND program
Run DOSS program
Run MAP program
Point the default web browser to the CRYSTAL web site
Open this help pdf file

Shows program and author's information

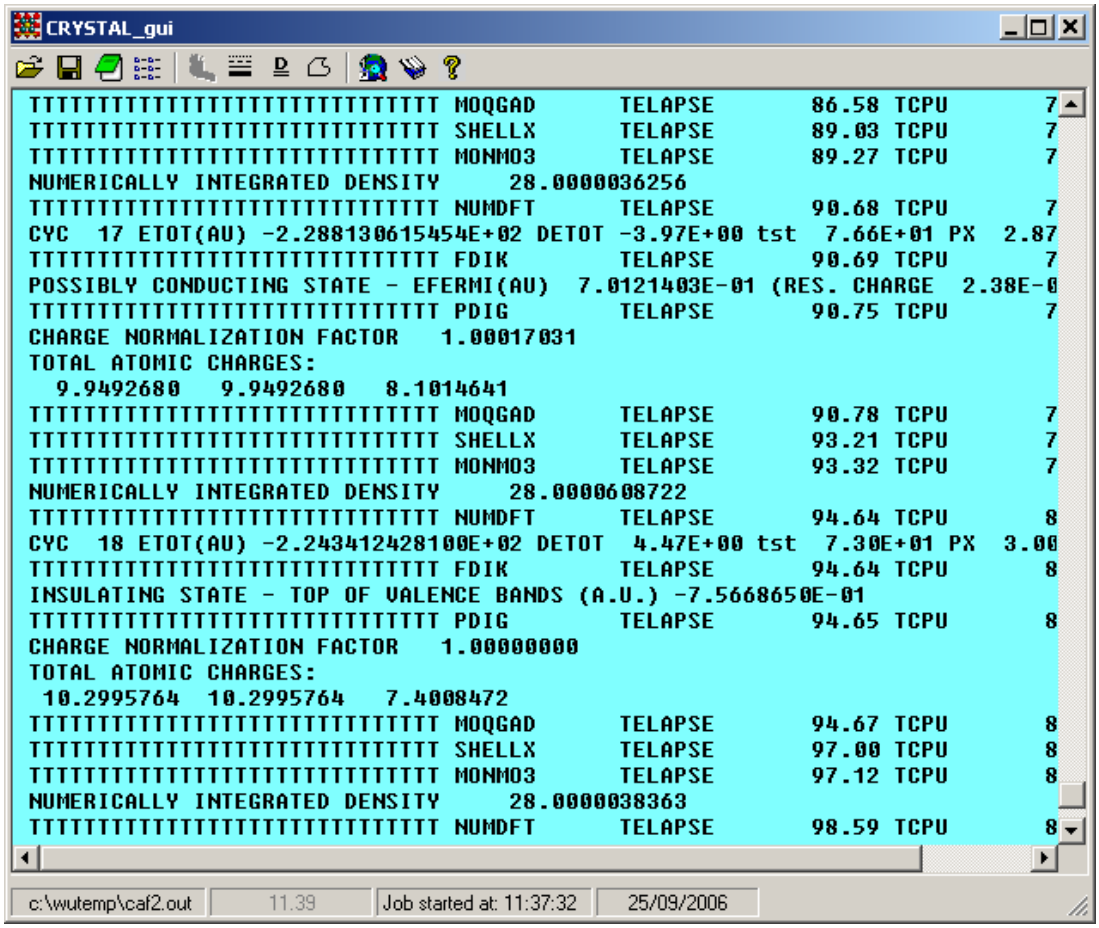
The first step is then to load a .d12 or .d3 file. The following window shows the case of test_standard.d12 (Magnesium oxide crystal):



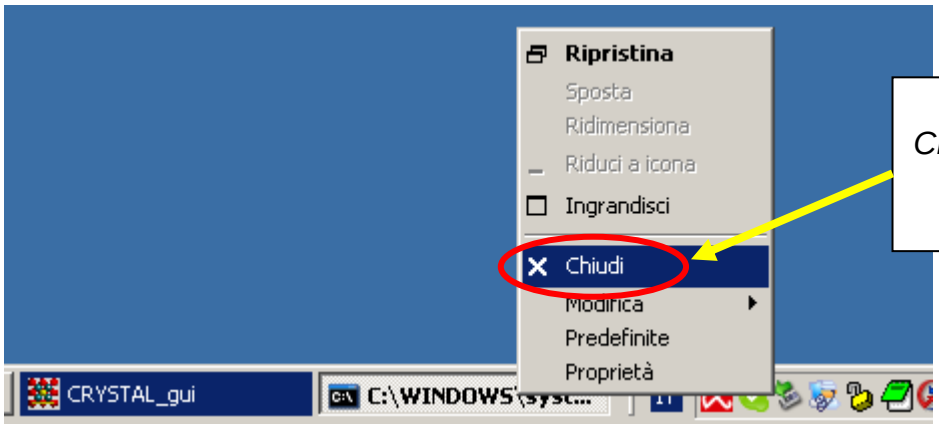
When the current .d12 file is submitted for execution a minimized run shell window will appear in the command bar:



Once the job is running the *CRYSTAL_gui* application cannot be closed and the control is passed to the CRYSTAL execution shell. The output file is captured by the *CRYSTAL_gui* interface (greenish background), it is regularly updated and can be scrolled up and down.



To kill the current job, simply right-click the CRYSTAL execution shell icon and select the "Close" option. The job will be immediately terminated and all files remain in place.



Result of right-clicking the CRYSTAL execution shell icon. Selecting "Close" will kill the current CRYSTAL run

If a file with the same name as the one submitted to CRYSTAL (for instance test.d12) but with .d3 extension is present in the same directory then *CRYSTAL_gui* will automatically launch the PROPERTIES calculation. At the end of the run, a check for the existence of unit fort.25 is performed and if found, MAPS, DOSS and BAND programs will be automatically launched as a function of the corresponding records written in the fort.25 file. If the user has previously installed the Ghostscript/Gsview programs and properly configured the crystal_gui.ini file then the Postscript file will be rendered on the screen.

MAPS, DOSS and BAND can also be launched separately once the unit fort.25 with the proper keywords is present in the actual directory.

The file crystal_gui.ini contains the names of various executables launched by *CRYSTAL_GUI* within the [executables_names] section.

```
;-----------------------------------------------------
; This is the CRYSTAL.INI file which is read
; by CRYSTAL_GUI.EXE at startup to set up
; executables names and future variables
;-----------------------------------------------------
[executables_names]
crystal_exe=crystal.exe
properties_exe=properties.exe
maps_exe=maps.exe
ps_exe=ps.exe
doss_exe=doss.exe
band_exe=band.exe
editor_exe=NotePad.exe
postscript_viewer=C:\Programmi\Ghostgum\gsview\gsview32.exe
```

Usually, the user is only concerned with two of them, namely the editor_exe and postscript_viewer ones.
The first one allows to specify the full path of the preferred text editor. The default is the windows notepad.exe. The second one allows *CRYSTAL_GUI* to automatically launch the postscript viewer. To view postscript output files you should visit the web site:

http://www.cs.wisc.edu/~ghost/doc/AFPL/get814.htm

and download both gs814w32.exe and gsv46w32.exe files and install them. Please note that release numbers (814, 46) may vary as a function of the software development. The keyword postscript_viewer in the [executables_names] section of the crystal_gui.ini file should then be set to the path where the viewer has been installed. For example:

[executables_names]
postscript_viewer=C:\Programmi\Ghostgum\gsview\gsview32.exe