Crgraph - 2006

Introduction

The package CrGraph-2006 processes data written by CRYSTAL06 in file fort.25 (saved by the execution script *runcry06* or *runprop06* as input_filename.f25), to give graphic outputs in postscript language.
Some records are written by CRYSTAL06 in a format different from CRYSTAL03 one.

```
BAND-DOSS-MAPN
1st record format: A3,I1,A4,2I5,1P,(3E12.5) - it was A3,I1,A4,2I4,1P,(3E12.5)

DOSS and BAND:
3rd record format: 6I5                          it was 6I3
```

The paper size is A4 (210x297 mm), in portrait mode. The maximum size of the plot is 180x270 mm.
The routines for plotting bands, maps and doss are antique and no authorship can be traced.
The present version is derived from a PC version implemented by Mauro Causà, and adapted with the insertion of the postscript driver by Ales Zupan.
B. Civalleri added the postscript to draw bonds and vdW spheres, deriving the program from MOLDRAW (P. Ugliengo).
Three Unix Cshell scripts are supplied to plot the computed data. They use environment variables defined bt cry2k6.cshrc
The argument identifies the input data. A default control data file may be supplied.

script name	plot type	input data	input control	default control	output	postscript
band06	band structure	$1.f25	$1.band	band.con	stdout	$1_band06.ps
doss06	density of states	$1.f25	$1.doss	doss.con	stdout	$1_doss06.ps
maps06	contour plot	$1.f25 $multi	$1.maps	maps.con multi.con	stdout	$1_maps06.ps

A specific meaning is attributed to some file extensions:

.f25	crystal data file (it may contain doss, bands, maps data)	input
.band	band structure control file	input
_band06.ps	band structure postscript file	output
.doss	density of states control file	input
_doss06.ps	density of states postscript file	output
.maps	contour maps control file	input
_maps06.ps	contour maps postscript file	output
.con	default control file (band.con, doss.con, maps.con)	input

Band structure - script: band06

Input control file: $1.band or band.con - Band data file: $1.f25

rec		variable	meaning
•	*	WDTH	width (mm) of the path in reciprocal lattice - max 180 mm
		HGTH	height (mm) of the energy axis - max 270 mm
•	*	NBMIN	index of the lowest band that can be plotted
		NBMX	index of the highest band that can be plotted
•	A	KLAB	label of the reciprocal lattice **k** vector axis
•	A	ELAB	label of the energy axis
•	*	EMIN	minimum value of the energy (Hartree) on the frame
		EMAX	maximum value of the energy (Hartree) on the frame
		DE	energy axis tick step (Hartree)
			insert 1 label per k-path segment extremes non coincident II
•	A	ILAB(I)	alphabetic character to identify the **k** point (Gamma for Γ, Delta for Δ, Lambda for Λ, Sigma for Σ)

Data to draw band structure are computed in *properties* by the keyword BAND, and are written in file $1.f25.
UHF calculation computes two sets of bands plotted in the same frame, and corresponding to α (solid line) and β electrons (dashed line).
The control file name is $1.band. When $1.band is missing, control data are input from band.con. The bands are plotted from EMIN to EMAX.
Warning The first band is the first band written for plotting (see BAND input, INZBN), not the lowest energy band of the system. It is recommended to write all the occupied bands computed + some virtuals, and choose the energy range to visualize when plotting.

Density of states - script: doss06

Input control file: $1.doss or doss.con - density of states data: $1.f25

rec		variable	meaning
•	*	WDTH	width (mm) of the energy axis - max 180 mm (equivalent to HGTH in band structure)
		HGTH	total height (mm) of doss axis - max 270 mm
•	*	EMIN	energy minimum value (Hartree)
		EMAX	energy maximum value (Hartree)
		DE	energy axis tick step
•	*	XPOS	relative coordinate (0.≤x≤1.) of the projection labelon energy axis
		YPOS	relative coordinate (0.≤x≤1.) of the projection label on doss axis
•	A	ELAB	label of the energy axis
			insert 2 records for each N-th doss projection - last projection: total doss II
•	*	SCALE	scale factor for the n-th projection
•	A	LBL	label for the n-th projection

UHF calculation computes two sets of density of states, corresponding to α (continuous line) and β electrons (dashed lines, with reverse sign). A scaling factor very large (50.) may be necessary to see some low density contributions (e.g. an electron localised in a lacuna).

Contour maps - script: maps06

Data to draw contour maps are computed in *properties* by the keywords ECHG, POTM, CLAS, and may be represented as total maps (1 set of data), standard difference maps (2 sets of data, in sequence in the same fortran unit 25), or maps of weighted superposition of CRYSTAL data obtained by different runs, computed in the same grid of points (see "multi").

Input control file: $1.maps or maps.con

rec	variable	meaning
• ∗	WDTH	width (mm) (A-B segment in CRYSTAL input) - max value 270 mm
	IROUTE	map type code: map / scale | linear | log | free | set(s) of data total | 0 | 2 | 4 | 1 difference | 1 | 3 | 5 | 2
	idraw	type of visualization: 0 | none 1 | atomic label 2 | stick 3 | ball and spockes 4 | vdW spheres
	color	0 | black and white postscript file 1 | color postscript file
		if IROUTE = 4 (or 5) — II
• ∗	FMIN	minimum value of the function
	FMAX	maximum value of the function
	DF	function increment between two contour lines

Continuous, dashed and dot-dashed lines correspond to positive, negative and zero values of the plotted function. UHF calculation produces two sets of data, computed from $\alpha+\beta$ (total) density and $\alpha-\beta$ (spin) density. Two maps are drawn in different pages when default scaling is chosen. Free scale generates linear increments of the function.

```
Default scale

Linear                                 |    Logarithmic - function values
             total     difference      |       total              difference
max value     0.1        0.015         |   0.2         E+2        0.2 0.4 0.8 E+1
min value    -0.1       -0.015         |   0.2 0.4 0.8 E+1        0.2 0.4 0.8 E+0
delta         0.01       0.001         |   0.2 0.4 0.8 E+0        0.2 0.4 0.8 E-1
                                       |   0.2 0.4 0.8 E-1        0.2 0.4 0.8 E-2
                                       |   0.2 0.4 0.8 E-2        0.2 0.4 0.8 E-3
```

if $1 equal 'multi'

1. define the environment variable *multi*, containing the list of the data files (without the suffix .f25). In cshell: `setenv␣multi␣'data1␣data2␣data3'`
2. prepare the file multi.con, following the attached instructions
3. prepare the file multi.maps with the plotting control instructions
4. give the command `maps␣multi`

Selection control file: multi.con

rec	variable	meaning
• ∗	NBLOCK	number of data block
		for each data block — II
• ∗	ISEQ	sequence number of the block in the data file obtained by attaching the files listed in $multi
	WEIGHT	weight of the block in the sum

Difference maps

The most common difference maps are used to show the influence of the crystal packing on the electron density:

- crystal versus atomic superposition:
  1 wave function calculation;

1 *properties* run, with the sequence: ECHG-PATO-ECHG (crys.f25);
1 maps run; the value of IROUTE in the control file must be odd.

- crystal versus superposition of non interacting molecules:
  1 wave function calculation for the crystal;
  1 *properties* calculation of the function of interest at grid points (crys.f25);
  1 wave function calculation for the periodic structure of non interacting molecules (keyword MOLSPLIT in geometry input);
  1 *properties* calculation of the function of interest at grid points (mol.f25).
  To obtain a differential plot (unix cshell):

  1. define the variable multi. In cshell: `setenv␣multi␣'crys␣mol'`;
  2. edit the file multi.con to define the selection and composition rules:
     ```
     2       two blocks of data to be summed up
     1  1.   the first block is the first in sequence, with weight 1.
     2 -1.   the second block is the second in sequence, with weight -1.
     ```
     a single block of data is obtained from the data: (1.*crys.f25) + (–1.*mol.f25).
  3. edit the plot control file multi.maps (IROUTE must be even). The simplest could be:
     `120 2 0 0` AB segment is 120 mm; logarithmic scale
  4. enter the command: `maps␣multi` . Needs the variable $multi, the files multi.con, multi.maps and the ones listed in $multi.

Appendix

The Crgraph package includes three plotting programs to process CRYSTAL data and two service programs, to select data from several files and to write a postscript file.

program	*properties* keyword	action
maps06.f	ECHG	contour maps of electron charge density
	CLASS	contour maps of classic electrostatic potential
	POTM	contour maps of electrostatic potential
band06.f	BAND	plotting of band structure
doss06.f	DOSS	plotting of density of states
sele06..f		selection of data from several CRYSTAL data
ps06.f		postscript driver

Each program selects the appropriate data from the file fort.25 by the program *properties* of CRYSTAL package. When files from different runs are used, the program **sele06.f** picks up the data of interesti (the script manages the call).
The three plotting programs write a temporary metafile, converted in a postscript file by the program **ps06.f**. All the programs use standard FORTRAN units and sequential data sets.

Installation

The crgra2006.tar file has to be expanded in the main directory of the CRYSTAL package. The directory crgra2006 should contain:

```
band06              cshell script to draw bands
doss06              cshell script to draw density of states
```

```
maps06              cshell script to draw contour maps
src/band06.f        fortran source
src/doss06.f
src/maps06.f
src/ps06.f
src/sele06.f
src/makefile
```

The following environment variables must be defined to create the executables and execute the scripts (they may be set by the shell cry2k6.cshrc):
CRY2K6_ROOT main directory of CRYSTAL package
CRY2K6_ARCH platform type (Release 2.0: Linux-pgf only) CRY2K6_GRA crgra2006 directory

The following fortran units are used during the execution:

fortran unit	written by	contents
25	***properties***	CRYSTAL data for plotting (read only)
19	***maps06.x***, ***doss06.x***, ***band06.x***	selected data for the plotted property
18	***maps06.x***, ***doss06.x***, ***band06.x***	metafile to be processed by ps06.x
21	***ps06.x***	postscript file