IRGrace

A Package for making a
grace file from data file

User's guide, IRGrace_12.1(Release 05.02.2012)
Morteza Jamal
Ghods City-Tehran-Iran
and
Ali H. Reshak
School of Complex Systems, FFWP-South Bohemia University, Nove Hrady 37333,
Czech Republic
School of Material Engineering, Malaysia University of Perlis, Malaysia

What is IRGrace?

IRGrace is a Package that helps you create a grace file from numerical data file

In order to use this Package the following public program packages must be installed :
  C-shell
  bc
Usually these public programs is available on Linux-systems.

This Package is the easiest way for making a grace file from data files and it can be very useful with xmgrace Package. It is sufficient use it for one time and you can understand why I say it is the easiest way for making a grace file.
Before using this package, I highly recommend provide a sheet and write in it informations about your frames and curves until you know what you want to plot and what informations you must to enter for your figs.

Copyright statement

Installation guide

If you want to install this package please follow the following steps.

Copy **"SRC_IRgrace.tar.gz"** file in your computer.
tar –zxvf SRC_IRgrace.tar.gz
cd SRC_IRgrace
run **"defbash_ir"** program (type **defbash_ir** in Terminal Environment).
This program add PATH of IRGrace in the **.bashrc** file. So, you can call it in any where.

Call Package

To call this Package it is sufficient call **Ginf_grace_ir** (type **Ginf_grace_ir** in Terminal Environment).

What does IRGrace do?

This package help you create a STYLE file called **PersianGulf.info** and a grace file with name **PersianGulf.agr** .Therefore you can use this STYLE file for other figs that you would like to have the same style but, with different data. After making grace file, you can see it with selecting **Plotting → View agr file** menu (if you have installed xmgrace Package).
You can get the newest informations about xmgrace and download it at the Grace home page http://plasma-gate.weizmann.ac.il/Grace/ .

For using this Package you must define ENVIRONMENT VARIABLE   called IRGRACE_PATH in your **.bashrc** file. Program **Defbash_ir** do that for you.
Moreover this program help Wien2k users plot Density Of States (DOS) easily. For plotting DOS file, use this command (**Ginf_grace_ir -dos**) for non spin-polarized system and (**Ginf_grace_ir -dos -up/-dn**) for spin-polarized system. Then when you select **Plotting → Specify files and columns to plot** menu and define PATH FILE FOR CURVE…… , this program reads informations of case.int file and shows them and you are able to select column to plot , exactly the same as dosplot2_lapw program.

This Package creates and shows grace file when you make changes in **PersianGulf.info** by using **Ginf_grace_ir** program and it closes xmgrace program (when it showes grace file) after 10 seconds if you run **checkXM_ir** in another terminal or in background of your system by using **at** command.

With this program, you are able to enter data from different path. I highly recommend use this program for making a grace file from a data file.

The JPEG and PNG output will be available, when you select **Plotting → Save**   menu, if additional libraries are installed when you install xmgrace. Those are:

The JPEG library ftp://ftp.uu.net/graphics/jpeg/ , version 6.x.
The PNG library http://www.libpng.org/pub/png/libpng.html , version 0.96 or above

xmgrace permits quite complex typesetting on a per string basis. For more informations see userguide of xmgrace and "**control codes**" table in userguide of xmgrace.

In IRGrace Package, if you want to write a word as superscript or subscript for X-label or Y-label or Curve label type as follows:
s for subscript , **S** for superscript, and **N** for normal type.
V**szz** = V$_{zz}$

V**Szz** = V^{zz}

P**s**xy**N**-As = P$_{xy}$-As

Moreover you are able to define different font (**f<name of font>**) such as Symbol as follows (you can see **window → Font tool** in xmgrace menus):
f<Symbol>d =
f<Symbol>D =
f<Symbol>D**f<>**n**s**d =   n$_d$ \\f<> = return to original font

\\f<x> = switch to font named "x"
\\f<n> = switch to font number n
\\f<>   = return to original font
\\R<x>= switch to color named "x"
\\R<n>= switch to color number n
\\R<> = return to original color
\\z<x> = zoom x times
\\z<>   = return to original zoom
\\r<x> = rotate by x degrees
…
…
…
…

Main Menu

  1- **Data**
  2- **Style**
  3- **X-axes**
  4- **Y-axes**
  5- **Font**
  6- **Plotting**
  7- **Add string**
  8- **Quit**

1- Data Menu
  1-1- *Specify frame Menu*

1-2- Specify curve
  Define number of curve in each frame.

1-3- Specify files and columns to plot
  Define PATH and name of file for getting data and columns to plot.

1-4- Quit
  For exit.

Specify frame Menu
  1-1-1- Specify number of frame (define number of frame)
  1-1-2- Specify title (define title for each frame)
  1-1-3- Specify subtitle (define subtitle for each frame)
  1-1-4- Specify view position by hand (define view position of frame)
  1-1-5- Specify view position automatically (define view position of frame)
  1-1-6- Quit (for exit)

2- Style Menu
  2-1- Specify line style
    Define line style

  2-2- Specify lines width
    Define line width

  2-3- Specify colors
    Define line color

  2-4- Specify symbols
    Define symbol to show numerical data

  2-5- Specify curve label
    Define label for curve

  2-6- Specify curve label position
    Define view position for curve label

  2-7- Quit
    For exit

3- X-axes Menu
  3-1- Specify label
    Define label for X-axes

  3-2- Specify scale
    Define scale for X-axes

3-3- Specify major tick
    Decide major tick for X-axes tobe On/Off and In/Out and then define color and distance between major tick

3-4- Specify minor tick
    Define number of minor tick between major tick and color for minor tick

3-5- Specify tick label
    Decide tick label for X-axes tobe On/Off and then define color for them

3-6- Quit
    For exit

4- Y-axes Menu
    It is the same as X-axes Menu

5- Font Menu
5-1- Specify font
    Define type of font

5-2- Specify font size
    Define size of font

5-3- Quit
    For exit

6- Plotting Menu
6-1- Create
    Creates grace file

6-2- View agr file
    Shows grace file by using xmgrace

6-3- Save
    Makes output (eps, png, jpeg) by using xmgrace

6-4- Quit
    For exit

7- Add string
   Define a string with special position, color, and degree

Ginf_grace_ir : This program gets informations and make STYLE file **(PersianGulf.info)** .

Cgrace_ir : This programs creates grace file **(PersianGulf.agr)** .

defbash_ir : Defines Environment Variable at the end of your **.bashrc** file.
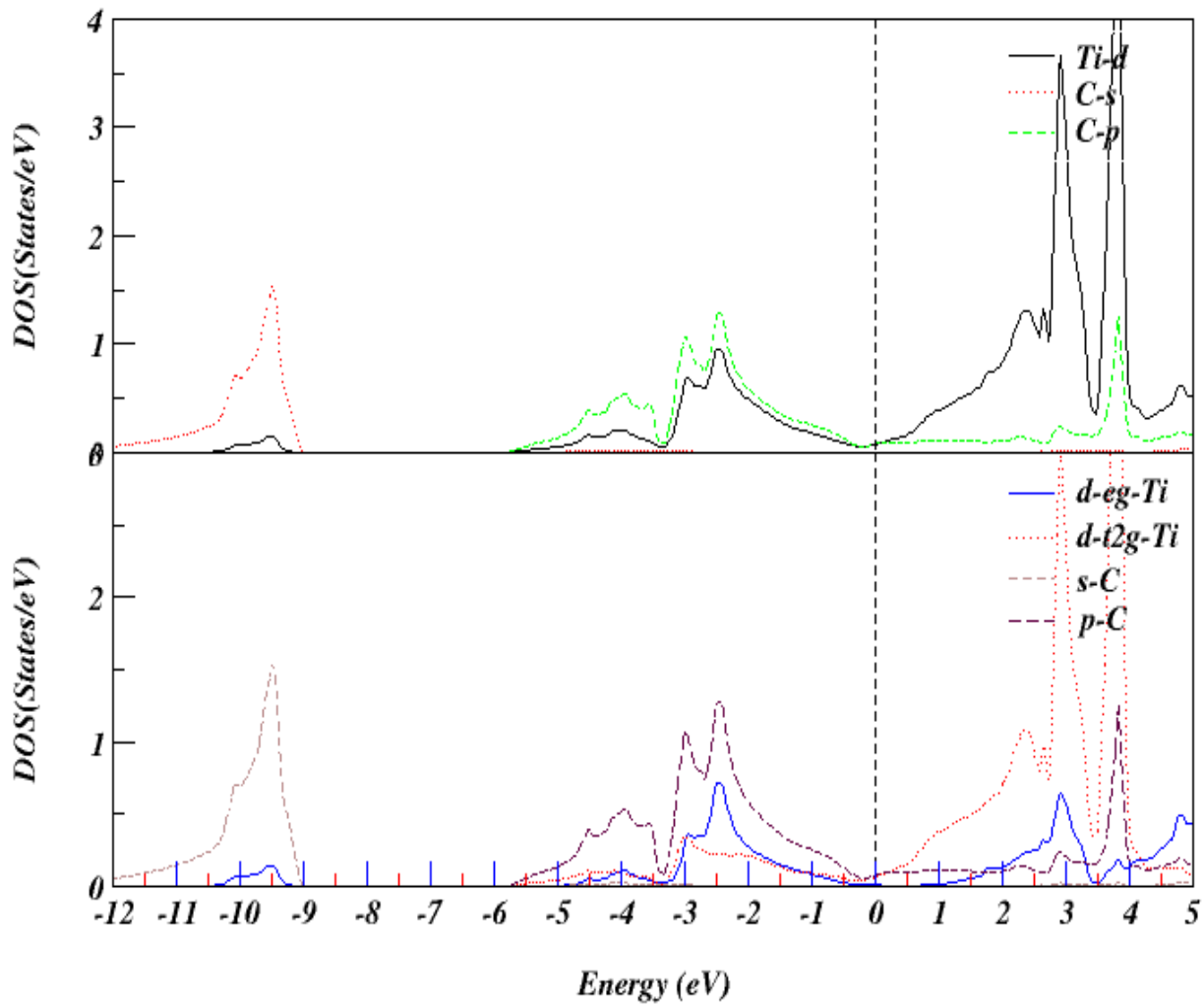
Deffun_ir: This program uses xmgrace program and with this program you are able to define a function for a curve.

Note: in this Package I have define the Xmgraxe window as follows:

(0.15,0.85)   (1.15,0.85)

(0.15,0.15)   (1.15,0.15)
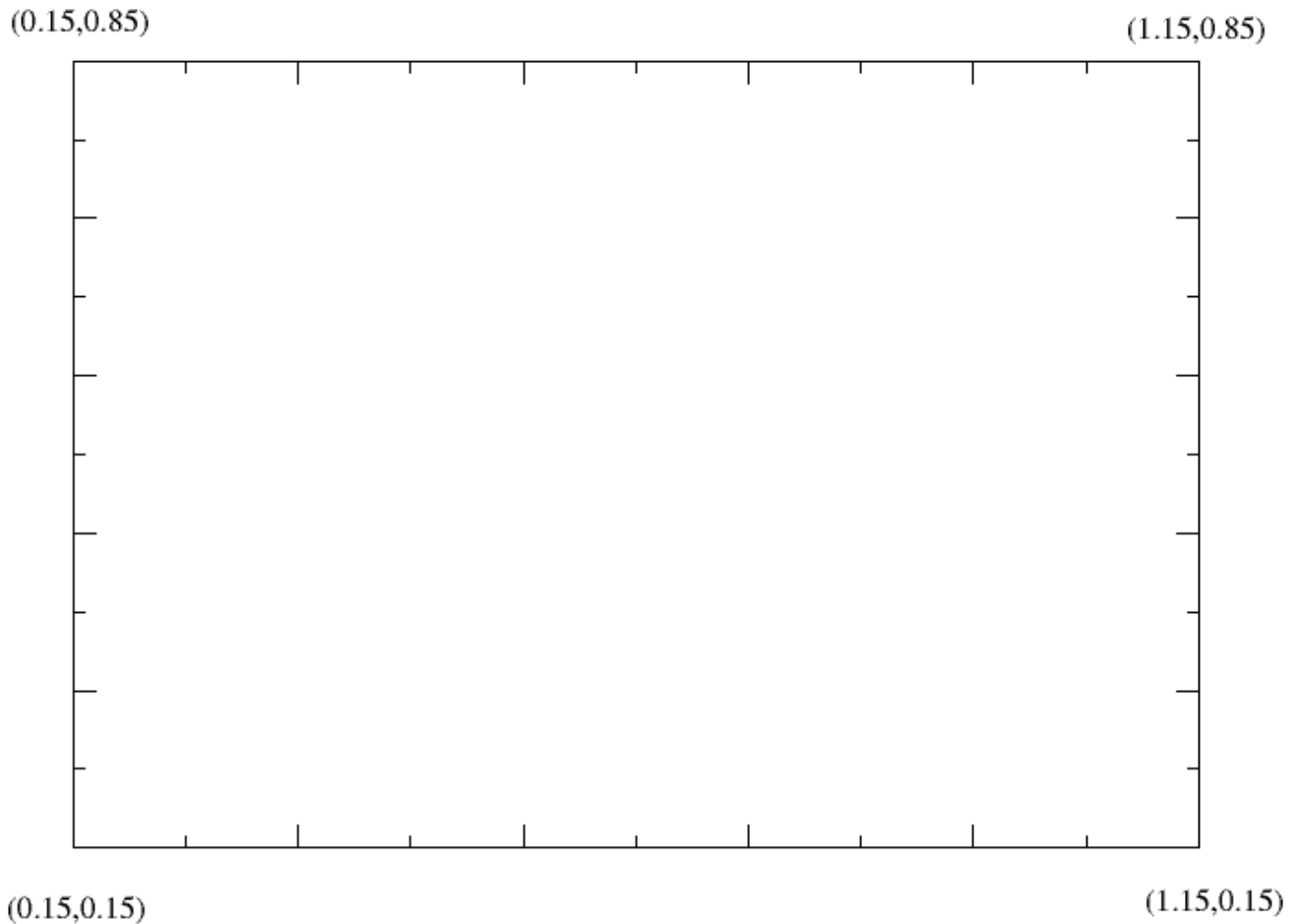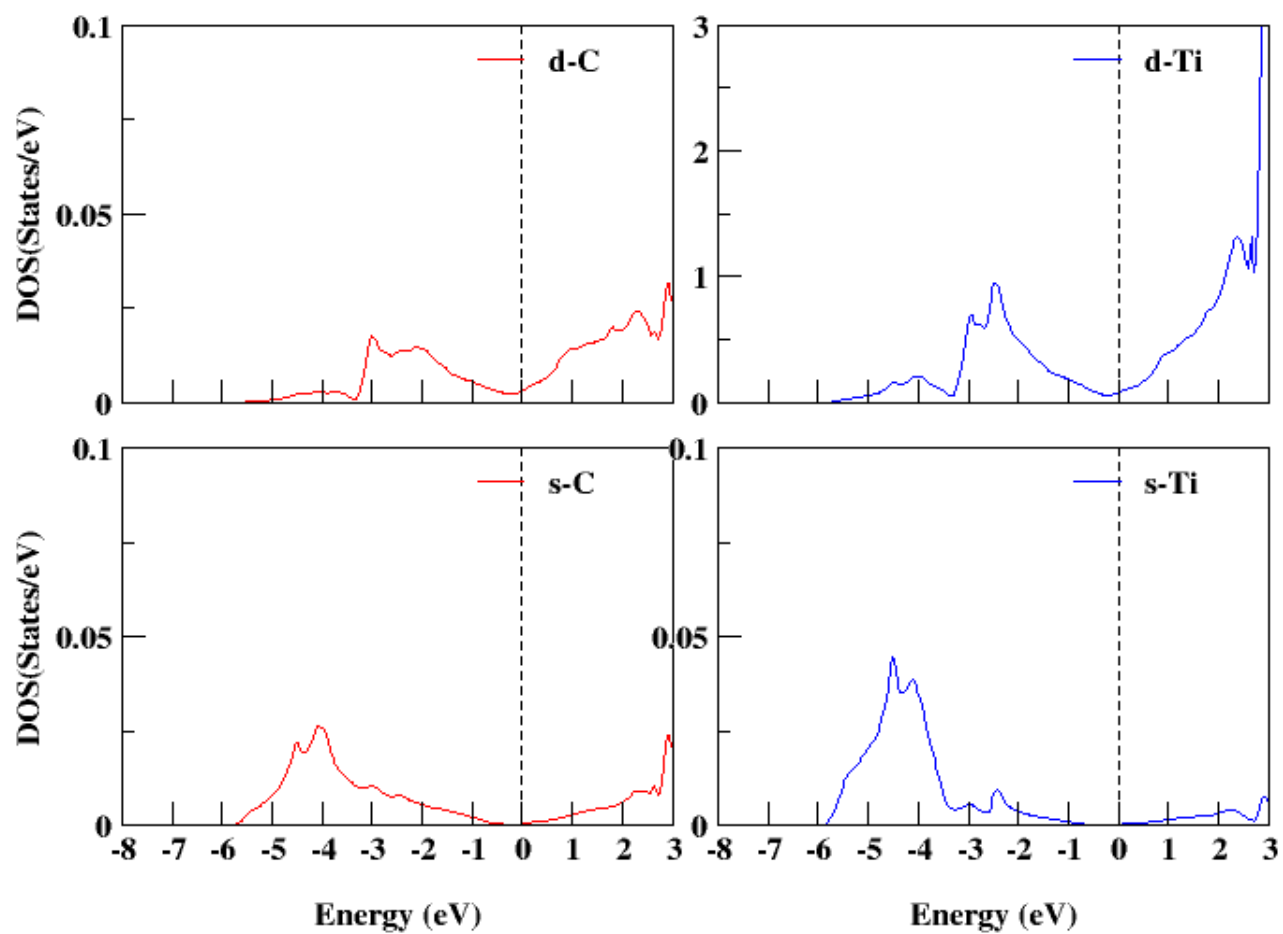
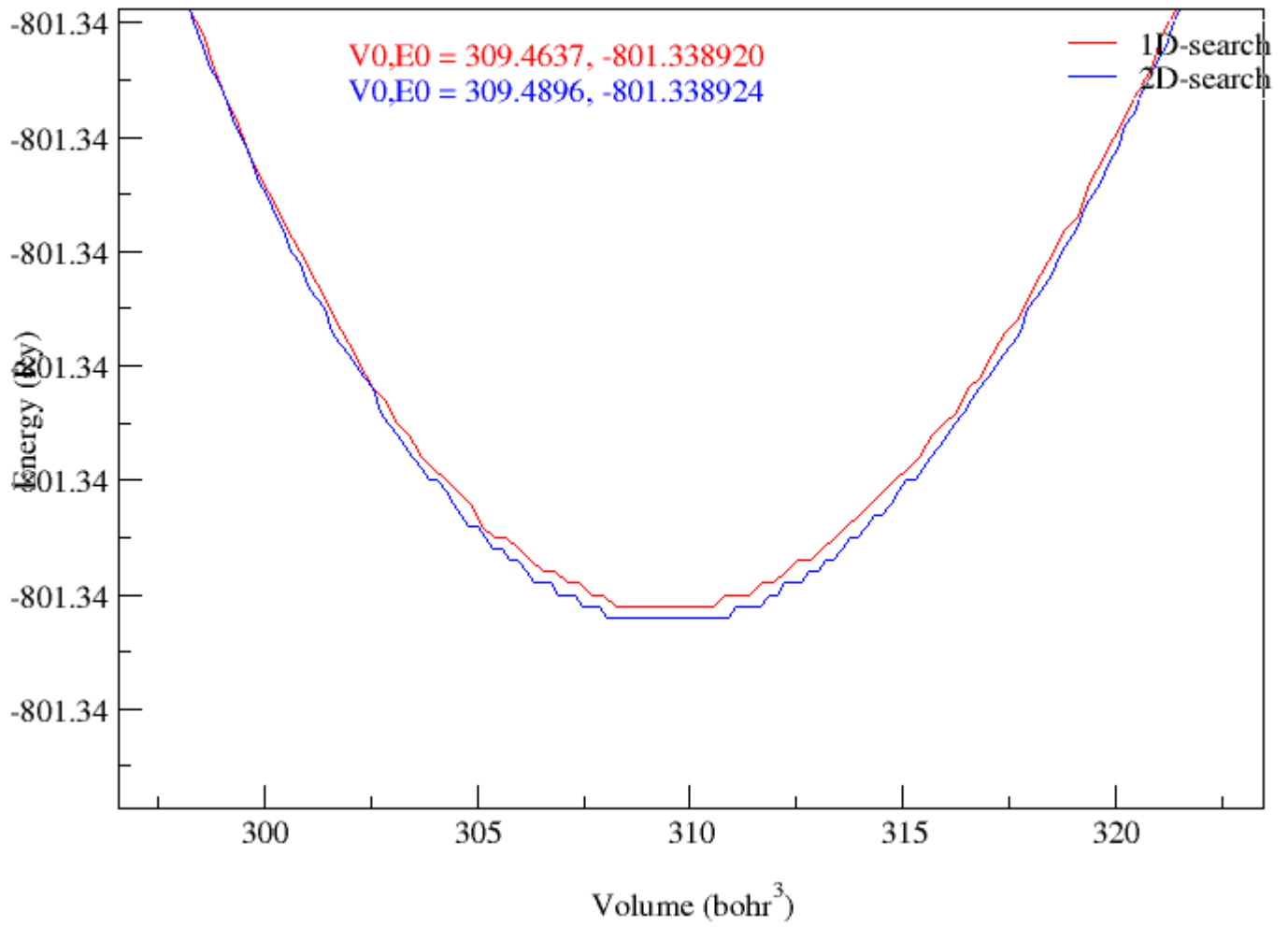**The following figs have been created by using this Package .**

TiC-DOS
Data-from-Wien2k

This plot has been created by using IRgrace and XMgrace

Equation Of State For hcp-Mg within GGA13

V0,E0 = 309.4637, -801.338920
V0,E0 = 309.4896, -801.338924

1D-search
2D-search

Energy (Ry)

Volume (bohr^3)