Fourier

Welcome

Fourier Program

A program for Fourier maps calculations.

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Introduction

The program ***Fourier*** calculates the scattering density inside the unit cell of a crystal of whatever symmetry. It uses a ***F***ast ***F***ourier ***T***ransform (***FFT***) subroutine to accelerate the calculation of the following expression:

$$\rho(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{H}} F(\mathbf{H}) \exp\left\{-2\pi i (\mathbf{H}\cdot\mathbf{r})\right\}$$

where V is the volume of the unit cell. $\boldsymbol{H}$ is a reciprocal lattice vector, $\boldsymbol{r}$ is a vector position inside the unit cell, and $F(\boldsymbol{H})$ are complex Fourier coefficients used to perform different types of Fourier syntheses. The units of $\rho(\boldsymbol{r})$ are those of $F(\boldsymbol{H})$ divided by those of V. For instance, if $F(\boldsymbol{H})$ are given en electron units (usual absolute units for X-ray diffraction) and V in $Å^3$, $\rho(\boldsymbol{r})$ is calculated as Number-of-Electrons / $Å^3$. In order to get absolute values of the density, the value of $F(000)$ should be provided (see F000 keyword).

Running the program

You can run ***Fourier*** from:

- Console
- by clicking on the  icon on the Toolbar of Fullprof Suite (***GFourier*** Program)

Console version

You can run ***Fourier*** from a console as follows:

Local_Prompt> *fourier [input_file] <cr>*

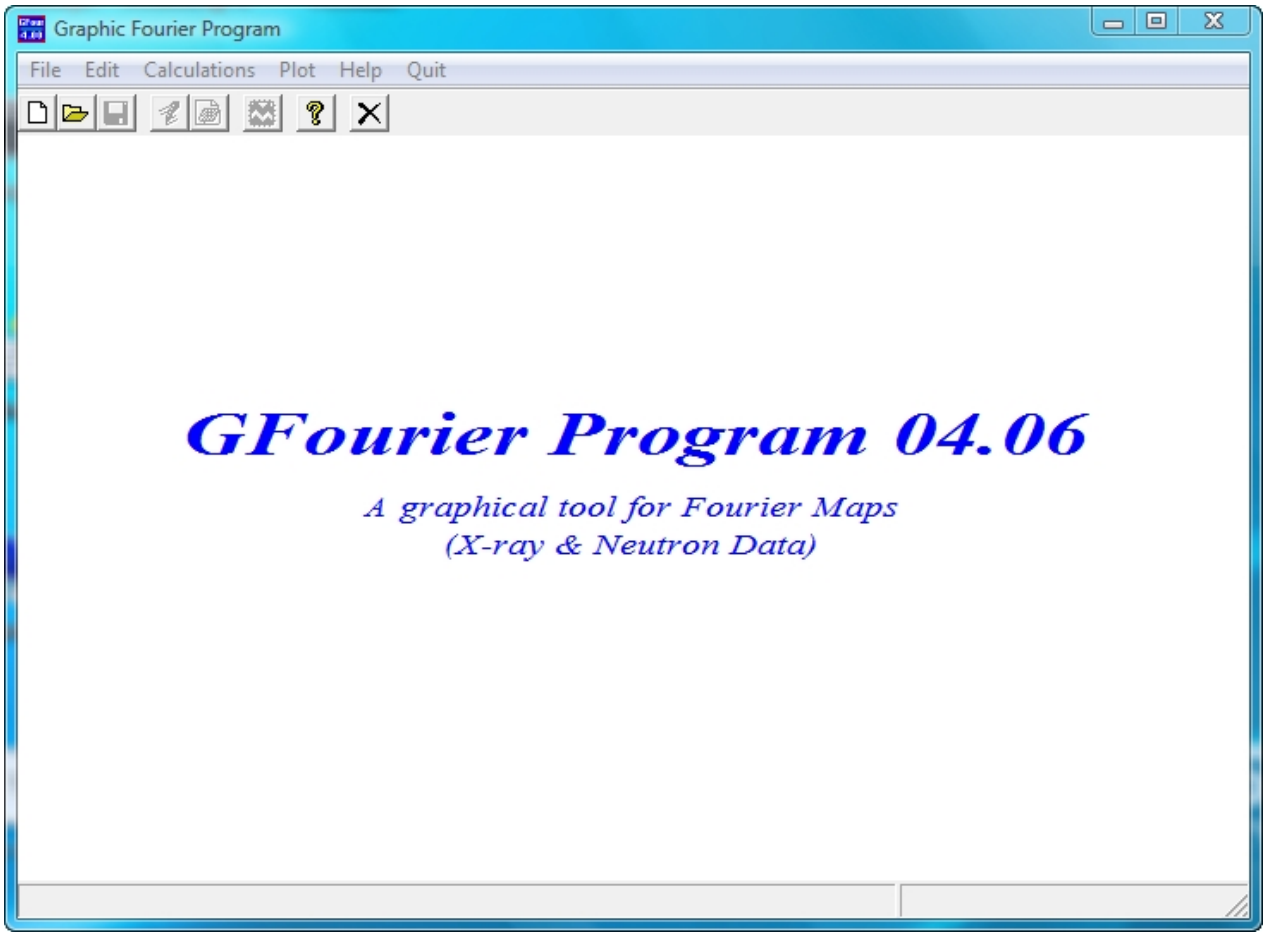
Input_File is the code of the input file summarizing the instructions for running ***Fourier***.

Also you need a file containing the hkl's and structure factors. The extension for both files are ***inp*** and ***fou*** respectively. If ***Fourier*** runs properly il will output up to two files:

CODE.fout General output file
CODE.bin Binary file containing the electron (or scattering) density inside the unit cell.

GFourier

The ***GFourier*** allows to create and visualise the results of ***Fourier*** program using a menu-driven interface with the help of the mouse and few keyboard input.



The program ***GFourier*** allows to create from the scratch an input control file **CODE.inp** for ***Fourier*** using just a menu-driven interface with the help of the mouse and few keyboard input. Before running the Fourier program after doing changes in GFourier it is necessary to save the file with the name of your choice, load it and then run the new calculations.

Input File

The input control file is totally free format. It is a command-driven-like file.

All commands and keywords are case insensitive. Empty lines are allowed and if the symbol "!" appears as the first character, the line is considered as a comment.

Keywords

The keywords are:

ATOM

ATOM *Label XYZ [Occ]*

Label	String (of 4 characters max) representing the name of the atom
XYZ	Three real numbers representing the fractional coordinates
Occ	Occupation number. (Optional parameter)

The atoms are not used for calculating the ***Fourier*** maps.They are given optionally only for graphic representation purposes or for distance and angle calculations. The program ***Fourier*** puts this information in the output binary file that is read by ***GFourier***.

Example: ATOM Ba 0.5000 0.5000 0.5000

CELL

CELL *a b c* α β γ

a	**a** parameter of the unit cell in Å
b	**b** parameter of the unit cell in Å
c	**c** parameter of the unit cell in Å
α	Alpha angle in º
β	Beta angle in º
γ	Gamma angle in º

Example: CELL 11.5378 6.2311 9.1344 90.0 90.0 90.0

END

END

This command tells the program that the lines below are not to be taken into account.

FILE

FILE *Keywords Namefile*

The command **FILE** provides information about files to the program. ***NameFile*** is the name of a file. It may include the full path.

The values of **Keywords** are:

Keywords	
FOU	The Structure factors file are provided in ***Namefile***
ATOM	Optional file for atoms is provided in ***Namefile***
BIN	Binary file with name ***Namefile***

NameFile can be absent if BIN and ATOM are given. In this case the name of the file is the same as the name of the input control file with extensions **.bin** and **.atm**.

Examples: FILE fou myfile.fou

FILE ATOM my_atoms.atm

FILE bin

FOURIER

FOURIER *Keywords*

This command tells to the program what kind of Fourier synthesis has to be calculated. At present, the possible values of **KeyWords** are:

PATT FOSQ	Patterson Map using observed squared structure factors	$F(\mathbf{H}) = \lvert F_{obs}(\mathbf{H})\rvert^2$
PATT FCAL	Patterson Map using calculated squared structure factors	$F(\mathbf{H}) = \lvert F_{cal}(\mathbf{H})\rvert^2$
FOBS	Fourier Map using observed structure factors and calculated phases	$F(\mathbf{H}) = \lvert F_{obs}(\mathbf{H})\rvert \exp\{i\varphi(\mathbf{H})\}$
FCAL	Fourier Map using calculated structure factors and phases	$F(\mathbf{H}) = \lvert F_{cal}(\mathbf{H})\rvert \exp\{i\varphi(\mathbf{H})\}$
DIFF	Difference Fourier Map	$F(\mathbf{H}) = \{\lvert F_{obs}(\mathbf{H})\rvert - \lvert F_{cal}(\mathbf{H})\rvert\} \exp\{i\varphi(\mathbf{H})\}$
AABB	User supplied real and imaginary parts of the Fourier coefficients	$F(\mathbf{H}) = A(\mathbf{H}) + iB(\mathbf{H})$

Examples:

FOURIER PATT FOSQ

FOURIER DIFF

The keyword FOBS can be supplemented with a second keyword like MSF or MEM. In the first case it means that magnetic structure factors are provided with its sign (coming from CCSL program Sorgam). In the second case a Maximum Entropy Map file will be used instead of calculating the Fourier Map. In this last cas it is expected also to provide the name of the file separated just by a space.

More Examples:

FOURIER FOBS msf

FOURIER FOBS mem my_maxent_file.mem

FORMAT

FORMAT *kw1 kw2 ... kw9*

Tells the program the order in which appear the different items in the Fourier file specified by FILE FOU. **kw (i)** are keywords representing one of the following items:

Examples:

FORMAT h k l A B

FORM h k l Fo Fc Phase

Form A B Fo h k l

F000

F000 *F000_value [Scale]*

Gives the value of F(000) and a scale factor for all map. The default values are F000_value=0.0000 and Scale=1.000

Example:

F000 822 1.0

GRID

GRID *nx ny nz*

User-supplied grid values for calculating the electron (or scattering) density. By default the program calculates automatically the three integer values **nx**, **ny** and **nz**.

Example:

GRID 20 20 25

LIST

LIST *Keywords*

This command instructs the program to output additional information. At present, the possible values of ***Keywords*** are:

ATOMS	List of atoms in the unit cell
DIST *value1 value2 value3*	List of distance of the peaks between value1 and value2. Value3 is the

maximum distance for angle calculations

In default, **value1** = 1.000, **value2** = 2.5 Å., **value3** = 0.0 Å.

Example:

LIST atoms

LIST dist 1.8 2.25 0.0

REFLEC

REFLEC *keyword Value(s)*

This command instructs the program about the sinθ/λ limits of Fourier calculation.

The ***Keyword*** is one of the items:

SRAN	*Value 1*	*Value2*	Range for sinθ/λ limits of Fourier calculation
SMIN	*Value1*		Minimum sinθ/λ limit of Fourier calculation
SMAX	*Value1*		Maximum sinθ/λ limit of Fourier calculation
SIGM	*Value1*		

Examples:

REFLEC SRAN 0.0 0.88

reflec SMAX 1.2

Reflec SMIN 0.2

SCAN

SCAN *npeaks*

This command activates the peak search procedure. The program looks for the coordinates of the highest ***npeaks*** peaks in the asymmetric unit of the |ρ(**r**)| map. These are repeated for the first ***npeaks*** peaks found. Symmetry equivalent peaks are not included.

Example:

SCAN 10

SPGR

SPGR *Space_Group*

The command **SPGR** tells to the program that the string ***Space_Group*** is the Hermann-Mauguin symbol for the space group. The symbol must be given using a space before the symbol corresponding to a symmetry direction. Following the International Table descriptions, choice 1 can be introduced by adding "**:1**" to Hermann-Mauguin symbol (choice 2 is in default) and for Rhombohedral axes "**:R**" (hexagonal axes are in default).

The program uses the symbol to generate the full set of symmetry operators that are used to expand the reflection indices. It is wise to verify that the reduced set of symmetry operators are correctly generated.

Examples:

SPGR P n m a

SPGR P 41/m

SPGR P m m n:1

SPGR R 3:R

TITLE

TITLE *Comment*

The command **TITLE** tells the program that comment should be used as a title.

Example:

TITLE Fourier Difference Map for CarboDiazepine