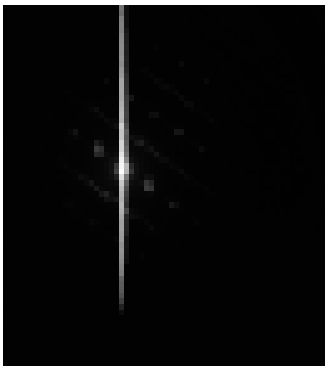
ELSTRU



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ELSTRU

Software Description
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Introduction

elstru is a program package to solve crystal structures from electrondiffraction data. The name of the program is a combination of ELECTRON and STRUCTURES, the Multi-Slice-Least-Squares (MSLS) is the heart of the system.

elstru is fully implemented on OpenVMS for Alpha. Limited version are available for different unix-flavours : Linux (Intel & Alpha) , IRIX , AIX and Tru64.Some

The features of elsim are:

-Contains all programs you need to refine a structure from scratch.

-Only one parameter file for all programs, which copes with all input not on the data files.

-Menu driven system to maintain the parameter file.

NOTE: This manual is experimentally. Please send all remarks to: joukj@hrem.stm.tudelft.nl.

The parameter file

All programs included in elstru are able to read their input from a parameter file, dgs.pf, or interactively from the terminal. The programs determine the input mode automatically by means of the following procedure:
-If the file dgs.pf does not exists in the current directory, terminal input is requested
-If the dgs.pf file is present the requested data is read from this file. However, if the data does not exists on the dgs.pf file, interactive input for the missing data is nescesarry.

The parameter file containsd lines according to the format:
varname = value \ any comment
varname is an expression of maximal 10 characters indicating the parameter name (i.e. the six parameters A, B, C, ALPHA, BETA, GAMMA indicate the crysltallographic unit cell). value is the value to be passed to the program on request for the parameter. It can be real, integer or characters, depending on the physical meaning of the parameter. After the back-slash any comment can be written.

Some of the programs calculate new values for parameters on the dgs.pf file. The file is then automatically updated.

The user can maintain the parameter file in three ways:
-Using a text editor
-Using the program PFILE
-Using the program PFMONITOR

The program GREED

Program name : GREED
Revision : 6.1
Systems : OpenVMS(Alpha), AIX(RS6000), IRIX6.2, Tru64, Linux(Intel & Alpha)
Pfmonitor command : greed , ?greed
Author : J.Jansen

Description
GREED is a general image/diffraction pattern imaging utility, which can do data-reduction on diffraction patterns. A tracer keeps continuously track of the current position on your data and the value of this point
A Menu is available for the tasks:
-EXIT GREED : exit the program
-change file ID : Change current file identification
-SCALE : Define a new scale for viewing. After selecting this option you have to select with your pointer a box within the image by clicking at two points.
-FLAT.CORR : Perform a flat-field correction.
-DIST.CALC : Calculate distance (in pixels of the CCD) of two points, pointed to by the pointer.
-LINE.CALC : Calculate equation of a line trough two points, pointed to by the pointer.
-LINE SCAN : Plots the profile along a line between two points, pointed to by the pointer.
-BOX INTENS : Total intensity within a box define by two points, pointed to by the pointer.
-DEF.EXCL.R. : Define excluded regions. Click at every corner of each region. A keystroke on the keyboard connects the first point and the last point and closes the current region. Several regions can be processed in a row.
-LOAD EXCL.R. : Load excluded regions from file
-AUTO EXCL.R. : Aoutomatic determination of excluded regions
-SAVE EXCL.R. : Save excluded regions to file
-PEAK SEARCH : Automatic peak search
-LOAD PEAK : Load peaks from file
-SAVE PEAK : Save peaks to file
-ADD PEAKS : Add peaks by clicking at the desired position
-REMOVE PEAKS : Clicking at a point in the image removes the nearest peak.
-RESET ORIGIN : With this option you can set the origin. In principle the peaksearch set the origin to the highest pixel in the image. However this fails if this pixel is within an excluded region.
-INDEX : Perform auto indexing on the peaks
-DATA REDUCTION : Determine integrated intensities of the indexed reflections.
-DEF TRANS : Define transfomation matrix
-TRANSFORM : Perfrom index transformation
-LOAD TRANS : Load transformation matrix from .ii file

-SHOW INDEX : Show indices of the location of mouse click.
-Def. Laue Circ. : Indicate the centre of the Laue circle with a mouse click. It is stored as the default value of the centre of Lauecircle after you do a TRANSFORM or DATA REDUCTION.
-PRINT : creates a post-script file of the image.
-refresh : Refreshes the screen by removing all lines that were drawn on the image.

Parameters required :

sendmail	Send E-mail to the one who runs the program with finishing status?
list	File to which all printable output should be routed. If @CONSOLE is given, the terminal screen is used for this purpose.
fileid	File identification used for constructiong automatic data-file extinctions
rdf	Image file name. If "@auto" is given files names derived from FILEID are used : <FILEID>_cor.dat or <FILEID>.dat. The "_cor" file is tried first. This is in principle the one corrected for the flatfield. If the the FLATFIELD option from the menu's is chosen always <FILEID>.dat is reopened. If greed does not auto-detect the data type DATA_TYPE, ENDIAN, DIMX, DIMY and OFFSET are used to read the data from file. Currently it reads the following formats: Tietz, Gatan2 & 3, Ditabis. If you specify greedstandard it can read many standard graphical files like TIFF,GIF,PNG,JPEG etc...
data_type	Date type image file w : 2-byte integers r : 4 byte reals c : 8 byte complex
endian	Big endian file? If the file is recorded on a Intel or Alpha system this should be answered NO. Else it is probably YES.
dimx	X-dimension image
dimy	Y-dimension image
offset	Offset of imagedata in bytes. Or with other words the length of the fileheader
exclf	Excluded regions file name If "@auto" is given files names derived from FILEID are used : <FILEID>.excl
pldevice	Plot device. At the moment only X11 is supported.
pvuf	Plot file name. In X11 mode it is used as window title.
plscl	Auto scale the image area?
plsxh	View port upper x. Determines x-coordinate of the upper right corner of the plot. for full size A4 20.0 is a reasonable value.
plsxl	View port lower x. Determines x-coordinate of the lower left corner of the plot. for full size A4 1.0 is a reasonable value.
plsyh	View port upper y. Determines y-coordinate of the upper right corner of the plot. for full size A4 20.0 is a reasonable value.
plsyl	View port lower y. Determines y-coordinate of the lower left corner of the plot. for full size A4 1.0 is a reasonable value.

plxmn	Minimal x to be processed (ignored if PLSCL="Y")
plxmx	"Maximal x to be processed (ignored if PLSCL="Y")
plymn	Minimal y to be processed (ignored if PLSCL="Y")
plymx	Maximal y to be processed (ignored if PLSCL="Y")
plhmx	Height corresponding to maximum intensity. This one is overruled if SCALE is selected from the menu's
plhmn	Height corresponding to minimum intensity. This one is overruled if SCALE is selected from the menu's
colourcode	Colour coding scheme. The default is *standard*
saturation	Colour saturation for the chosen colour scheme
c_invert	Invert colour coding scheme? Normally this is NO.
numcell_x	Number of cells x-direction to be viewed for diffraction patterns a number not equal to 1 does not make sense.
numcell_y	Number of cells y-direction to be viewed for diffraction patterns a number not equal to 1 does not make sense.
cph	Phase colour coding in a cyclic way for compex images?
rdfnew	New raw image file name after flatfiled correction. If "@auto" is given files names derived from FILEID are used : <FILEID>_cor.dat
flatf	Flatfield file name
rest_bg	Restore background level after flatfield correction?
satlev	The value above which your CCD is saturated
gapval	Gap value. This should be a value which does not appear in your data (i.e. -100000.)
do	Interpolation method for peak search P : Polynomial G : Centre of gravitation S : Spline interpolation (recommended)
noisemul	Noise multiplication factor. This parameter is important to detect the correct peaks in the peaksearch. a too low value gives rise to many ghost peaks. If the value is too high many peaks are missed. A good value is about 10.0.
peakf	Peak file name containing the peaks after a peak search. If "@auto" is given files names derived from FILEID are used : <FILEID>.pek
spsigma	Spline tension (For spline interpolation) the recomended value is 1.0.
autoindex	Automatic indexing? recommend is "Y". If this parameter is "N" then the origin, the 100 and the 010 reflection have to be pointed to using the pointer.
handindex	Hand indexing? If autoindex is switched off and this one is switch on you have to give indices for all peaks you select. If switched off you have to select the origin and the ends of the two reciprocal vectors that span the zone.
degree	Degree of index fit. In our experience 3 is the best value.
indperdeg	Indices per degree before degree higher. Usually this parameter is set to something like 20000. Lower it when indexing fails.
orig_x	X-coordinate origin (if indexing is done only)
orig_y	Y-coordinate origin (if indexing is done only)
indexf	name of file containing the indexing information. If "@auto"

	is given files names derived from FILEID are used : <FILEID>.index
ang_min	Minimal reciprocal cell angle allowed for indexing. A good value is 30.
fom_max	maximal Figure Of Merit to accept cell dimensions. A good value is 0.1.
wavel	Wavelength of radiation
cammlength	Cammera length in mm. This parameter is used to calculate the cell dimensions from CCD-pixels
pixsize	CCD pixel size in mm. This parameter is used to calculate the cell dimensions from CCD-pixels
use_centr	Use central beam? Currently it is not advised to use the central beam.
hmin	Minimal h-index used in data-reduction
hmin	Maximal h-index used in data-reduction
kmin	Minimal k-index used in data-reduction
kmax	Maximal k-index used in data-reduction
squar_box	y : square boxes in data reduction. n : circular boxes in data reduction.
use_fit	Use fit for saturated pixels? Replace the oversaturated pixels in a peak by the ones which are calculated from a fit of a Gaussian peakshape to the non-oversaturated part of the paek. Note that you cannot use this option if you have use the *Auto exclude* option in GREED.
show_fit	Show fitted peaks in 3D-plots? Use this option for debugging only.
use_fitbac	Use background fitting and not one geussed from the edges of the picture during datareduction. This option is still experimental, but it looks promissing when turned on.
hklif	HKI file name. If "@auto" is given files names derived from FILEID are used : <FILEID>.ii
ermult	Error multiplication factor. Determines if an intensity is significant I>ermult*sigma(I). Normally a value 2.0 will do.
a	Cell axis A
b	Cell axis B
gamma	Gamma
title	Observation title (part 1)
title1	Observation title (part 2)
samtitle	Sample identification
printf	This file name is used to write PostScript to when the PRINT option is selected from the menu.

The program IMVIEW

Program name : IMVIEW
Revision : 7.0
Systems : OpenVMS(Alpha), AIX(RS6000)
Pfmonitor command : imview , ?imview
Author : J.Jansen

Description
Imview is a general image/diffraction pattern imaging utility A tracer keeps continuously track of the current position on your data and the value of this point
A Menu is available for the tasks:
-EXIT IMVIEW : exit the program
-FILES : read a new file using a menu driven file browser. Click on the file to select or click <new> or <previous> for other files. Click <cancel> to keep the old file. Note that this option does not work well with the automatic filename generation in the data-reduction part. It is not recomended to use this option for quick previewing of the files only.
-SCALE : Define a new scale for viewing. After selecting this option you have to select with your pointer a box within the image by clicking at two points.
-DIST.CALC : Calculate distance (in pixels of the CCD) of two points, pointed to by the pointer.
-LINE.CALC : Calculate equation of a line trough two points, pointed to by the pointer.
-LINE SCAN : Plots the profile along a line between two points, pointed to by the pointer.
-BOX INTENS : Total intensity within a box define by two points, pointed to by the pointer.
-PRINT : creates a post-script file of the image.

Parameters required :

list	File to which all printable output should be routed. If @CONSOLE is given, the terminal screen is used for this purpose.
fileid	File identification used for constructiong automatic data-file extinctions
series	Series of images? Normally this is answered with "N". "Y" is only experementally yet
rdf	Image file name. If "@auto" is given files names derived from FILEID are used : <FILEID>_cor.dat or <FILEID>.dat. The "_cor" file is tried first. This is in principle the one corrected for the flatfield. If the the FLATFIELD option from the menu's is chosen always <FILEID>.dat is reopened.
rdf*	Raw data image file name * to be used if a series is viewed
pldevice	Plot device. At the moment only X11 is supported.

pvuf	Plot file name. In X11 mode it is used as window title.
plscl	Auto scale the image area?
plsxh	View port upper x. Determines x-coordinate of the upper right corner of the plot. for full size A4 20.0 is a reasonable value.
plsxl	View port lower x. Determines x-coordinate of the lower left corner of the plot. for full size A4 1.0 is a reasonable value.
plsyh	View port upper y. Determines y-coordinate of the upper right corner of the plot. for full size A4 20.0 is a reasonable value.
plsyl	View port lower y. Determines y-coordinate of the lower left corner of the plot. for full size A4 1.0 is a reasonable value.
plxmn	Minimal x to be processed (ignored if PLSCL="Y")
plxmx	"Maximal x to be processed (ignored if PLSCL="Y")
plymn	Minimal y to be processed (ignored if PLSCL="Y")
plymx	Maximal y to be processed (ignored if PLSCL="Y")
plhmx	Height corresponding to maximum intensity. This one is overruled if SCALE is selected from the menu's
plhmn	Height corresponding to minimum intensity. This one is overruled if SCALE is selected from the menu's
rdfnew	New raw image file name after flatfiled correction. If "@auto" is given files names derived from FILEID are used : <FILEID>_cor.dat

The program MSLS

Program name : MSLS
Revision : 16.5
Systems : OpenVMS(Alpha), AIX(RS6000), IRIX6.2, Tru64, Linux(Intel & Alpha)
Pfmonitor command : msls , ?msls
Author : J.Jansen

Description
The Multi-Slice Least-Squares program MSLS is designed to refine crystallographic parameters, such as coordinates, temperature factors, occupancies, crystal thickness and crystal orientation, from electron diffraction data. The data reduction to get the initial HKLI-files should be performed using the program GREED and the files with atomic position can be made either by the programs ATOMS or XATOMS.

Parameters required :

sendmail	Send E-mail to the one who runs the program with finishing status?
list	File to which all printable output should be routed. If @CONSOLE is given, the terminal screen is used for this purpose.
rfacsumf	File to write R-factory summary to.
groupno	Space group number according to *The International Tables for X-Ray Crystallography* volume A. If spacegroup 0 is specified the name in SPGROUP is used. If that fails it is ussumed that the parameters LATTICE, NEQV, CENT and SYM* describe the symmetry.
setting	Space group setting as in *The International Tables for X-Ray Crystallography* volume A.
spgroup	Spacegroup name: i.e. P212121. If this name is @NUM the spacegroup number is used.
lattice	Lattice type according to space group. Possibilities: P, A, B, C, I, F, R.
cent	Centro symetrical unitcell?
neqv	Number of equivalent general atom positions. Pairs of centro symmetric positions count as one.
sym*	(* = 1,2,3,...24) The symmetry opperations. The number of operations is determined by the parameter neqv. Examples of these operations are: x,y,z 1/2-x,y+3/4,-z
fl_ep	Flack like absolute structure parameter
a	Crystallographic unit cell a-axis
b	Crystallographic unit cell a-axis
c	Crystallographic unit cell a-axis
alpha	Crystallographic unit cell α-angle
beta	Crystallographic unit cell β-angle
gamma	Crystallographic unit cell γ-angle
fdimx	Fourier dimension x-direction. 0 gives the default of 128

fdimy	Fourier dimension y-direction. 0 gives the default of 128
optim_sl	Optimal slice size in Ångstrom for the Multi-Slice calculation.
atomf	File containing the initial atomic parameters
newatomf	New atom file name
constrf	File containing the constraints. If no constraints are wanted give NL: for this parameter. The file should contain lines in the form: p(<atname>)=p(<atname>)*r+p(<atname>)*r-p(<atnam e>)+r where p = one of: x : x-coordinate y : y-coordinate z : z-coordinate b : Temperature factor o : Occupancy and <atname> is the atomic identifier. An example is : x(Ba1)=y(Ba2)*2.0-.5 The lines are case insensitive and blanks are ignored.
ref_x	Refine x-coordinates?
ref_y	Refine y-coordinates?
ref_z	Refine z-coordinates?
ref_b	Refine temperature factors?
ref_occ	Refine occupancies?
ref_abso	Refine absorption factor?
ref_thick	Refine thickness?
ref_laue	Refine Centre of Laue circle?
ref_to	Refine overall Debye-Waller factor?
ref_abss	Refine absolute structure parameters?
ref_twin	Refine twinning parameters?
to	Overall temperature factor
scatype	Scattering factor type B : Bird and King C : Cromer & Mann (+Moth formula) D : Doyle and Turner (Use with care) F : (Fails) I : Waasmaier & Kirfel (+Moth formula) K : Kirkland P : Peng R : Rez & Rez & Grant (+Moth formula) W : Weickenmeier
modfres	Use modifies Fresnel propagator? (NEVER TESTED IF TRUE)
absorb	Absorbtion parameter
dampfac	Damping factor. Normally .5-.75 The actual damping factor applied to the shifts is this averall damping multiplied by the parameter specific one (i.e. dampfac_c for atomic coordinates.) normally the atomic specific damping factors are set to 1.0, unless some parameters give rise to an instable refinement.
dampfac_s	Damping factor scales
dampfac_t	Damping factor thickness

dampfac_l	Damping factor Lauecircle
dampfac_c	Damping factor coordinates
dampfac_b	Damping factor temperature factors
dampfac_o	Damping factor occupancies
dampfac_e	Damping factor absolute structure parameters
dampfac_a	Damping factor absorbtion factors
numcyc	Number of refinement cycles
autothick	use autothickness determination
thick_strt	Start thickness for auto thickness determination
thick_end	End thickness for auto thickness determination
thick_step	Thickness step for autothickness determination
absslauestp	Use absolute laue steps? (or use two dimensional vectors related to the indexing vectors of greed?)
laue1hstep	first Laue_step H-direction
laue1kstep	first Laue_step K-direction
laue1lstep	first Laue_step L-direction
laue2hstep	second Laue_step H-direction
laue2kstep	second Laue_step K-direction
laue2lstep	secon Laue_step L-direction
lstep1min	Minimum multiplication Laue step 1
lstep1max	Maximum multiplication Laue step 1
lstep2min	Minimum multiplication Laue step 2
lstep2max	Maximum multiplication Laue step 2
idiff	I-differnces file (NL: no file). This parameter is for testing purposes
all_ref	Use Rcode=2 reflections in refinement? Normal value is "N"
rcode_list	if not all rcodes ar used this variable listts the rcodes to be used
excelf	Henny's EXCEL name. If NL: or if it is left blank no file is written.
pr_refm	Print refinement matrix?
ref_on_i	Refinement based on intensities? if not square roots of intensities are used.
swap_i_f	Toggle refinement basis from intensities to squareroot intensities and vice versa every n th cycle.
use_centr	Use central beam in the refinement?
min_d	Minimal d-value of the reflections to be used. Normally this value is set to 0.0.
hklif<n>	Hkli-file name <n> (<n> = " " , "1" , "2" ,...)
hklif<n>new	New Hkli-file name <n> (<n> = " " , "1" , "2" ,...) This file is updated with phases.
use_set<n>	Use the Hkli-file no <n> (<n> = " " , "1" , "2" ,...) in this refinement.
crysize<n>	Thickness <n> (<n> = " " , "1" , "2" ,...)
nsubsl<n>	Number of sub-slices <n> (<n> = " " , "1" , "2" ,...)
laue_c_h<n>	Centre of the Laue circle h <n> (<n> = " " , "1" , "2" ,...)
laue_c_k<n>	Centre of the Laue circle k <n> (<n> = " " , "1" , "2" ,...)
laue_c_l<n>	Centre of the Laue circle l <n> (<n> = " " , "1" , "2" ,...)

ref_laue<n>	Refine Centre of Laue circle for dataset <>n? (<n> = "0" , "1" , "2" , ...)
ref_twin<n>	Refine twin parameter for dataset <n>? (<n> = "0" , "1" , "2" , ...)
twin_par<n>	Twin parameter for dataset <n>. (<n> = " " , "1" , "2" , ...)
t_mat11_<n>	Twin matrix(1,1) for dataset <n>. (<n> = " " , "1" , "2" , ...)
t_mat12_<n>	Twin matrix(1,2) for dataset <n>. (<n> = " " , "1" , "2" , ...)
t_mat13_<n>	Twin matrix(1,3) for dataset <n>. (<n> = " " , "1" , "2" , ...)
t_mat21_<n>	Twin matrix(1,1) for dataset <n>. (<n> = " " , "1" , "2" , ...)
t_mat22_<n>	Twin matrix(2,2) for dataset <n>. (<n> = " " , "1" , "2" , ...)
t_mat23_<n>	Twin matrix(2,3) for dataset <n>. (<n> = " " , "1" , "2" , ...)
t_mat31_<n>	Twin matrix(3,1) for dataset <n>. (<n> = " " , "1" , "2" , ...)
t_mat32_<n>	Twin matrix(3,2) for dataset <n>. (<n> = " " , "1" , "2" , ...)
t_mat33_<n>	Twin matrix(3,3) for dataset <n>. (<n> = " " , "1" , "2" , ...)
scalefac<n>	Scaling factor <n> (<n> = " " , "1" , "2" ,...). A good starting value is 1.0.

The program PFILE

Program name : PF
Revision : 2.0
Systems : VAX/VMS, ULTRIX, AIX(370), AIX(RS6000)
Script : pf.com
Author : J.Jansen

Description
PFILE is a program to help viewing and changing the parameter file dgs.pf. The program should be used running the script pf.com.

On VMS systems a variable on the parameter file can be examined by:
@PF.COM variable
On UNIX systems this will be
PF.COM variable

To change a variable on a VMS system
@PF.COM variable=value
and on UNIX systems
PF.COM variable=value

The program PFMONITOR

Program name : PFMONITOR
Revision : 9.2
Systems : OpenVMS for Alpha, AIX(RS6000), Linux(Intel & Alpha), Irix, Tru64
Author : J.Jansen

Description
The purpose of this monitor is to create an environment in which all parameters that are used by the powder analysis programs are defined. The parameters can be assigned a value and then passed to a specific task, that upon completion will update the value of the appropriate parameters in the monitor, thus allowing you to chain a number of tasks where the input for one is ,at least inpart, provided by the output of the previous task.

In order to run the monitor program on a OpenVMS system the command should be installed by the PFMONITOR.CLD file. i.e. On the VAXcluster at the laboratory for crystallography of the university of Amsterdam this can be done with the command:
SET COMMAND $DISK2:[JOUKJ.COM]PFMONITOR This command can be inserted in the users LOGIN.COM.
ON AIX for RS6000 the program works properly for a VT220 terminal only. so insert in your .cshrc (for csh) the command:
set term=vt220

You can start the monitor by typing either "pf" for the *old* user-interface or "pf /WX" for the current user-interface.

The Extended Backus Naur Formalism (EBNF) is used to describe the syntax of PF command lines. EBNF provides some rather simple rules to define a syntactic entititie. Say in defining an entitie A, the line

A ::= B	states that the entitie A is legally represented by B
A ::= B|C|D	means that A can be either B, C or D, | denotes a choice
A ::= (B|C)|D	is equivalent to line above, () is used to group subexpressions
A ::= [E]	A can be E or empty, ie. represented by nothing at all
A ::= {F}	A is either empty, or composed of any number of concatenated F's, ie. F FF FFF etc.
A ::= {"{"}	legal A's are { {{ , " is used give a EBNF metacharacter its literal, uniterpreted meaning

For example, defining A ::= [BC]{,(DE)}F, then among all concatenations that match this definition are
B,D,E,D,E,D,E,DF ,D,D,D,DF C,E,E,E,EF

The monitor is driven by command lines. The general syntax of a commandline is :

commandline ::= keyword[/l] argument { ,argument } { |keyword[/l] argument { ,argument } }

A keyword consists of a string of characters, the first of which must be a letter, to be defined as :
keyword ::= identifier
identifier ::= letter{letterdigit}
letter ::= a..zA..Z$?_
digit ::= 0..9
Keywords are userdefinable, and once known to PF, they are recognised by their shortest, unique abbrevation. A keyword belongs to just one of the following classes : command, process, function, macro or parameter. This class determines a keyword's global properties as well as the syntax and semantics of its argument(s). Keywords are assigned a class by a class-id (cid) in the define command.

Some definitions:

command	perform a monitor specific action, like show or change the value of a parameter, define a new keyword, terminate the execution of pf.
process	schedule a new task, passing(c) or not passing(p) it the value of all defined parameters and do(c) or do not(p) update the parameters depending on this tasks output.
function	a standard function, to be used in an expression.
macro	a named entity in which a number of command lines can be stored, and be executed by name.
parameter	a variable that can be assigned a value and that is accessible by a process scheduled from the monitor.

Any keyword is associated with a certain class when it is defined. A cid is identified by a single character :

p	process
m	macro
x	command
u	function
f	function
c	process

Several cid's are used to specify the class parameter, each indicating a different data type :

i	integer
r	real
b	A filename
s	character
l	character*1

An explanation of all classes follows.

COMMAND classid : x
definition command : define x keyword expression
PF can perform a number of intrinsic commands, mainly to alter and inform the user on, its global state. The command actions itself are not, however the

name by which a certain command is invoked, is userdefinable.
The action associated with a command name is defined by the value of the expression, this must be an integer in the range 1..17. Upon scheduling of the monitor, the only command defined is the define command itself, all other commands are then defined and named from the initialisation file, default pf.init. The following commands are implemented:

bye	1	terminate, optionally save current state
close	2	close list or audit file
define	3	create a new keyword
delete	4	delete a keyword from PF's database
describe	5	list the class and value of a (group) of keywords
detach	15	create a detached process
convex	16	Routes the job to a CONVEX machine via COVUEBATCH
help	6	provide help on a keyword or defined helpitem
null	-	do nothing command, an empty command line executes this command
open	7	open a list or audit file
process	8	writes parameters to parameter file, spawns a dcl process, reads the parameter file.
prompt	9	prompt at the console for a keyword value
read	10	read a diskfile, and execute all commands it contains
run	14	Spawns a process and does not wait to finish it.
spawn	11	spawns a dcl command
type	12	list the value of an expression
uh	13	read the universal header of a PHILIPS powder diffraction datafile
wuh	16	writes several parameters to the universal header of a PHILIPS powder diffraction datafile

MACRO classid : m
definition command ::= define m keyword
macrobody
>
invocation command ::= keyword argumentlist
argumentlist ::= [argument]{,argument}
argument ::= char{char}'(' argumentlist ')'
char ::= any character, execpt a comma (',')
The macro body can contain any number of legal PF command lines, the definition is completed by a >, this must be the first character on a new line (rest of that line is ignored).
In the macro body formal (dummy) arguments of the format %i% or %i-%, where i is an integer constant in. When executing the macro, these formal parameters will be replaced by actual parameters in the commandline, where %1% corresponds to the first actual parameter, %1-% to all parameters from the first, %2% to the second etc. If no actual parameter corresponds to %i%, %i% represents a null string, that is it is completedly ignored.

FUNCTION classid : u or f
definition command : define u|f keyword expression
classid u : user defined function. The expression is an real expression. %1% is the function parameter

f : Standard function. The expression solves to the function code
A function keyword may be used in an expression. When used in an expression, the argument list of the function MUST be delimited by (and), EVEN WHEN THE ARGUMENTLIST IS EMPTY.
The standard functions with their function codes are:

abs	1	Absolute value
acos	2	Inverse cosinus in radials
acosd	3	Inverse cosinus in degrees
asin	4	Inverse sinus in radials
asind	5	Inverse sinus in degrees
atan	6	Inverse tangens in radials
atand	7	Inverse tangens in degrees
cos	8	cosinus in radials
cosd	9	cosinus in degrees
cosh	10	Hyperbolic cosinus
exp	11	Exponential function
log	12	Natural logarithm
log10	13	Logarithm based on the value 10.
sin	14	Sinus in radials
sind	15	Sinus in degrees
sinh	16	Hyperbolic sinus
sqr	17	Square-function
sqrt	18	Square root
tan	19	Tangens in radials
tand	20	Tangens in degrees
tanh	21	Hyperbolic tangens

PROCESS classid : p or c
definition command : define p|c keyword dclcom
dclcom : An expression resolving to the dcl command of the process to be scheduled by this keyword.
classid c : The parameters are written to the parameter file first and updated after executing the dcl command
classid p : the dcl command is executed with the old parameter file
A once defined process can be scheduled by typing the command line : keyword { argument } where the optional argument comprises literally ALL of the rest of the line entered. It's the new processes responsability to pick up this line and interpret it.

PARAMETER
definition command ::= define tid keyword
tid ::= i|r|l|s
The datatype of a parameter is set by the tid letter you use in the definition.
i - integer data, range aprox -10^9..10^9 (32 bits two's complement)
r - real data, range approx. -1.0e-38.. 1.0e+38, internal precision about 7 digits
s - string, a string of maximally 80 ascii characters.
l - character , a string of one character All keywords defined as parameter are accessible by son-processes run by PFMONITOR, through the so called parameterfile created before a proces is invoked.

EXPRESSION
PFMONITOR will evaluate expressions like 5+3-2 and (7.1 + 5)*(3 -2.9). Defined keywords can be used in an expression, (aap+noot) \ mies will be evaluated using the current value of these three keywords, provided these were defined. The type of an expression's value is cast to that of the resulting variable Formal syntax of PF expression :

		examples
expression	::= [|-][term] { (+|-) term }	\ -5 + 3
term	::= factor { (*|/) factor }	\ 2*3^5*8/3
factor	::= efactor { ^ efactor }	\ aap^3.4
efactor	::= constant | keyword | "(" expression ")"	\ 2 noot (3.1\2.2)
constant	::= integer|real|string	\
integer	::= digit{digit}	\ 1234 9876
real	::= digit{digit}.{digit}[(E|e)(+|-)digit[digit]	
string	::= "{char}"	\ "a*b.c@d=e"
digit	::= 0|1|2|3|4|5|6|7|8|9	\
char	::= any character from ASCII characterset.	

If you include an optional /l switch on a keyword, all output (except error messages) will be appended on the current listfile. The range of this switch is limited to the scope of the keyword invoked. If you use the switch on a macro keyword or on the read command, then the action of the switch will extent to all commands executed in the macrobody or the inputfile read.
Initially the listfile will be the same as the outputfile, usually your terminal, in this configuration the l switch has no noticable effect.
To get output on a file, not the console, first use the 'open list filename' command.
!!! NB! A parameter, named list is defined in the default file file pf.init for Powder diffraction and pf_e.init for electron diffraction. This parameter is passed to the diffraction programs scheduled from PF, its value is totally independed from the listfile you open in PF itself. The PF listfile and the file named in the parameter list can however be identical

The program XATOMS

Program name : XATOMS
Revision : 5.1
Systems : OpenVMS(Alpha), AIX(RS6000), IRIX6.2, Linux(Intel & Alpha), Tru64
Pfmonitor command : xatoms , ?xatoms
Author : J.Jansen

Description
X-windows interface to edit the atomic parameters.
The colour codings are as follows :
brown : name
blue : refinable parameter
red : fixed parameter
green : constraint parameter
cyan : unchangeble by this program.
A Menu is available for the tasks:
-EXIT : exit the program (Note that this option does NOT save the changes)
-Save atoms : creates a new atomic parameters
-Add atoms : Adds an atom. Give the name, x, y, z and B separated by a press of <RETURN>.
-Insert atoms : click on the location where to add a new atom. then procede as with the add-option.
-Change values : click on place to change and correct.
-Toggle fix : click on a field to toggle between fixed and refineable parameters.
-Delete atom : Click on the atom to be deleted
-Copy atoms : Select atoms to copy to the paste-buffer.
-Cut atoms : Select atoms to be moved to the paste buffer.
-Paste atoms : Copy the contents of the paste buffer to the given location.
-aniso <-> iso B : Toggle a atom between isotropic and anisotropic Debye-Waller factors by clicking on the atom.
-Special options : edit special atom options like rigid body gragment number and sphere shell radius
-Add constraint : Select atom and add the contraint
-edit contraint : Click on a green value and change the constraint
-del. constraint : Remove the constraint from the selected parameters.
-Next atoms : next screen with atoms
-Previous atoms : Previous screen with atoms
-shift atoms : Apply the same translation to all atoms.
-Rotate atoms : Apply a rotation to the all the atoms.
-Transform atoms : apply a certain matrix transformation to the atom positions.
-calc. proj.pot. : view the current projected potential for the requested zone orientation.

Parameters required :
sendmail Send E-mail to the one who runs the program with finishing status?

list	File to which all printable output should be routed. If @CONSOLE is given, the terminal screen is used for this purpose.
groupno	Space group number according to *The International Tables for X-Ray Crystallography* volume A. If spacegroup 0 is specified the name in SPGROUP is used. If that fails it is ussumed that the parameters LATTICE, NEQV, CENT and SYM* describe the symmetry.
setting	Space group setting as in *The International Tables for X-Ray Crystallography* volume A.
spgroup	Spacegroup name: i.e. P212121. If this name is @NUM the spacegroup number is used.
lattice	Lattice type according to space group. Possibilities: P, A, B, C, I, F, R.
cent	Centro symetrical unitcell?
neqv	Number of equivalent general atom positions. Pairs of centro symmetric positions count as one.
sym*	(* = 1,2,3,...24) The symmetry opperations. The number of operations is determined by the parameter neqv. Examples of these operations are: x,y,z 1/2-x,y+3/4,-z
num_atset	Atomic dataset to be used. Normally this number is 1.
atomf	Atom file
newatomf	New atom file
atomf1	Atom file for atomic set no. 2
newatomf1	New atom file for atomic set no. 2
constrf	File containing the constraints
newconstrf	New file containing the constraints
plsxh	View port upper x. Determines x-coordinate of the upper right corner of the plot. for full size A4 24.0 is a reasonable value.
plsxl	View port lower x. Determines x-coordinate of the lower left corner of the plot. for full size A4 2.0 is a reasonable value.
plsyh	View port upper y. Determines y-coordinate of the upper right corner of the plot. for full size A4 20.0 is a reasonable value.
plsyl	View port lower y. Determines y-coordinate of the lower left corner of the plot. for full size A4 2.0 is a reasonable value.
a	Crystallographic unit cell a-axis
b	Crystallographic unit cell a-axis
c	Crystallographic unit cell a-axis
alpha	Crystallographic unit cell α-angle
beta	Crystallographic unit cell β-angle
gamma	Crystallographic unit cell γ-angle
fdimx	Fourier dimension x-direction. 0 gives the default of 128
fdimy	Fourier dimension y-direction. 0 gives the default of 128
to	Overall temperature factor
scatype	Scattering factor type B : Bird and King C : Cromer & Mann (+Moth formula) D : Doyle and Turner (Use with care) F : (Fails) I : Waasmaier & Kirfel (+Moth formula)

K : Kirkland
P : Peng
R : Rez & Rez & Grant (+Moth formula)

numcell_x	Number of unitcell of projected potential in x-direction to be viewed
numcell_y	Number of unitcell of projected potential in y-direction to be viewed