

ConfPlot

Version 2.4

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Introduction

ConfPlot is a program for visualising a configuration of atoms used for example by Reverse Monte Carlo (RMC) simulations. Although there are advanced programs available for this purpose we feel that it is practical to have a free and simple program that runs on a PC under Window95/NT or any other system. This program uses the graphical library PGPLOT from T.J.Pearson [1]. It also uses the PGXTAL package for 3-D rendering developed by D.S.Sivia [2].

To compile and link ConfPlot 2.0 you need the following files:

PGPLOT: pgplot.lib, rgb.txt, grfont.dat, grpkg1.inc (rgb.txt and grfont.dat should be included in directory c:\pgplot).

PGXTAL: pgxtal.f .

CONFLOT: ConfPlot (main), AddList, DelList, Determ, ErrorColour, ErrorType, FindCommand, FindDirection, FixDens, GetCol, GetDens, GetMatrix, GetView, Help, Initiate, OpenRead (system dependent), ReadConfig, SetAtoms, SetBonds, SetBox, SetColours, SetCut, SetDotSpins, SetSpins, SetSurface, SetupPrint, SetupScreen, SplitFile, SplitString, Transf, Transform, TransformAll, ucase.

Make sure you have the correct version of OpenRead, there is one for windows and one system independent version.

Changes from version 2.0:

- CPLOT shift fixed
- PGPLOT Windows metrics fixed
- Histogram options added
- Rmcplot options added
- Colour or grey-scale density plots
- Cursor mode to read off co-ordinates and distances in plots
- Dot-product colour-mapped "bonds"
- Co-ordination polyhedra plots
- Nested command file calls and parameter passing
- Explicit set-up of plot page size and plot area
- Symmetrisation of density plots using space-group operators

Plot types

The program reads an atomic configuration from a file with extension .cfg. The format of this file should be the same as used by the Reverse Monte Carlo program RMCA [3]. You can also read from a configuration that contains spin directions as coordinates instead of positions.

ConfPlot reads a number of commands from the keyboard to change colours, views,... etc. There are four kinds of plots, which can be displayed by ConfPlot.

1. Atoms as spheres at the position given in the configuration file.

Atoms represented as spheres, each atom type can have a colour and radius that you choose. Atoms can also be connected with bonds. The command for this kind of plot is PLOT.

2. Spins as arrows.

Arrows representing spin orientations can be plotted at positions given in a configuration file. The spin (arrow) directions have to be read from a spin file (with the same format as the configuration file). The command for this type of plot is SPLOT.

Atomic density plots.

A crystallographic configuration contains many unit-cells. To get a better illustration of disorder in such configuration, it is possible to shift each cell into one unit-cell. The atom positions in such merged cell can then be represent as "atomic density" or probability to find an atom. ConfPlot use a 3-D grid of the (merged) cell to calculate this "atomic density". Two types of plots can be made on "atomic density".

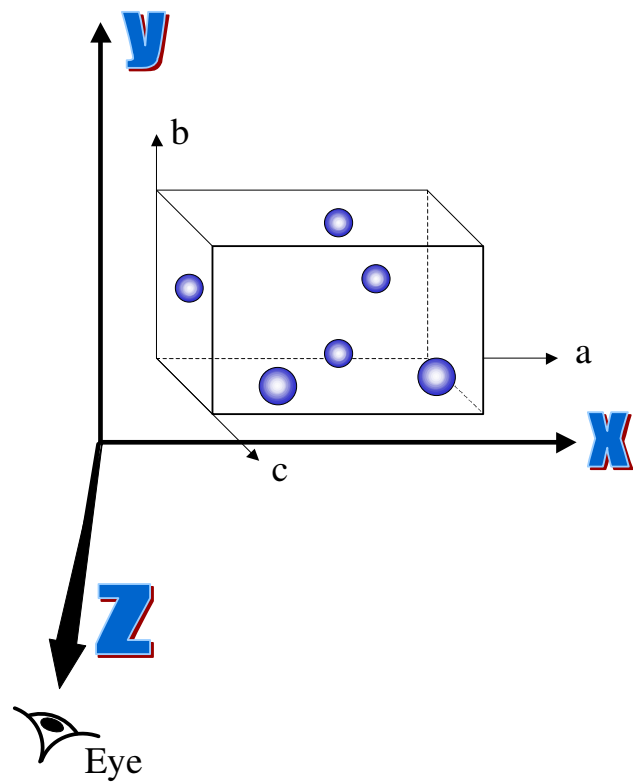
3. 3-D surface at a given atomic density in the cell.

A surface wrapped around a region with constant "atomic density" can be made with the command DPLOT. Each region (atom type) can have it's own colour and surface density chosen by the user.

4. 2-D "contour" plot in a plane that cut through the cell.

A 2-D "contour"-plot (colour-scaled) of the "atomic density" can be made with the command CPLOT. The plot will present the density in an arbitrary plane cutting through the cell.

Commands given to ConfPlot are not case sensitive and it is only necessary to give the first characters of the command for ConfPlot to recognise the command (i.e. "background" give the same result as "ba"). The configuration is plotted in a Cartesian coordinate system (x -, y - and z -axis) with the positive z -axis pointing towards you.



Command Table:

Command	Argument [optional]	Description
ARROW	[<i>arad alen</i>]	Define shape of arrays used in spin plotting SPLOT. Radius <i>arad</i> and length <i>alen</i> (Å). Default values <i>arad</i> =0.1 <i>alen</i> =1.5 Å.
ATOM	<i>itype</i> [<i>icolour</i>]	Used to give the atom type <i>itype</i> the colour represented by index <i>icolour</i> (see colour index list) and/or to make the atom type visible. (The default colours are set by the colour index list).
NOATOM	<i>itype1</i> [<i>itype2</i> [...]]	Make atom type(s) <i>itype1</i> [<i>itype2</i> [...]] invisible.
BACKGROUND	<i>icolour</i>	Set background colour to the colour represented by index <i>icolour</i> (see colour index list). Default background is black.
BOND	<i>itype1 itype2 rmin rmax</i>	Plot bonds between atoms of types <i>itype1</i> and <i>itype2</i> if the distances between the atoms are greater than <i>rmin</i> and less than <i>rmax</i> . Default bond colour is blue.
NOBOND	[<i>itype1 itype2</i>]	Deletes bonds between atoms of types <i>itype1</i> and <i>itype2</i> . If no arguments are given then all bonds are deleted.
BOX	[<i>icolour</i> [<i>lab</i>]]	Plot a cell box with the colour represented by the index <i>icolour</i> (see colour index list) and/or make the box visible. Default box colour is white. You can label the axis by setting <i>lab</i> =1 (default <i>lab</i> =0 no labelling).
NOBOX		Make the cell box invisible.
CBW		Make contour plots using grey-scale
CCOLOUR	[<i>icolour1</i> [<i>icolour2</i> ...]]	Make contour plots using colour maps. Optionally use colours <i>icolour</i> ...Default colours are blue-cyan-green-yellow-red.
CDENSITY	<i>dlow dhigh</i>	Set density limits <i>dlow</i> and <i>dhigh</i> for visible atoms (given by ATOM/NOATOM) type. This is used to set the borders of the 'contour'-plot created by CPLOT. If <i>dlow</i> or <i>dhigh</i> < 0, the limits will be set automatically.
CPLOT	[<i>mgn</i>]	Plot a 'contour'-plot of the atomic density, in a plane through the cell. The plane orientation can be changed by CUT, and the 'contour' limits by CDENSITY. A magnification of the plot can be set by <i>mgn</i> . Default value for <i>mgn</i> = 1. (The colours does not depend on settings by ATOM, only the visibility can be changed by ATOM/NOATOM.)

CURSOR		Toggle using cursor ON/OFF in plot windows. When cursor is ON coordinates and distances can be displayed by left-clicking in the plot window.
CUT	<i>aa bb cc na nb nc</i>	Define the plane through the cell used by CPLOT to make a 'contour'-plot. (<i>aa,bb,cc</i>) give a point within the plane. (<i>na,nb,nc</i>) give the normal to the plane. $0 \leq aa,bb,cc \leq 1$. Default values are: (<i>aa,bb,cc</i>) = (0.5,0.5,0.5), (<i>na,nb,nc</i>) = (0,0,1). These values are also used by the SLICE command (see below).
DENSITY	<i>itype dens</i>	Set surface density <i>dens</i> for atom type <i>itype</i> used by DPLOT. The region is opaque for atom density $> dens$ and transparent for atom density $< dens$. If $dens < 0$ the surface density will be set automatically.
DIRECTION	<i>nva nvb nvc</i>	Rotate the configuration box so that it will be viewed from direction (<i>nva, nvb, nvc</i>). Default is (0, 0, 1), look along the c-axis.
DOTBOND	<i>itype1 itype2 rmin rmax [dmin dmax]</i>	Plot dot product colour mapped bonds between <i>magnetic</i> atoms of types <i>itype1</i> and <i>itype2</i> if the distances between the atoms are greater than <i>rmin</i> and less than <i>rmax</i> . Bond colours depends on the current colour map and the value of the <i>relative</i> dot product of the pairs of spins. If <i>dmin</i> and <i>dmax</i> are given only bonds with dotproduct between <i>dmin</i> and <i>dmax</i> are plotted. Default values are <i>dmin</i> = -1 and <i>dmax</i> = +1.
NODOTBOND		Deletes dot product bonds between atoms of types <i>itype1</i> and <i>itype2</i> . If no arguments are given then all dot product bonds are deleted.
DOTPRODUCT	<i>a b c [dmin dmax]</i>	Calculate the dot product between direction (<i>a,b,c</i>) and each spin. Spin arrows will be plotted if their dot product with (<i>a,b,c</i>) lies between <i>dmin</i> and <i>dmax</i> . $-1 \leq dmin < dmax \leq +1$. Default values are (<i>a,b,c</i>)=(1,0,0), <i>dmin</i> = -1 and <i>dmax</i> = +1.
DPLOT	[<i>mgn</i>]	Plot a 3-D surface around a constant atomic density. The surface density can be changed by DENSITY. This command is usually used after merging the configuration with UNITCELL. A magnification of the plot can be set by <i>mgn</i> . Default value for <i>mgn</i> = 1.
END		Used in command files to exit the command file execution and return to a higher level or the ConfPlot command prompt.
EXIT/QUIT		Exit the program.
FRAME	[<i>fxmin fxmax fymin fymin</i>]	Define plot area in fractional units of the page size (see PAGE command). Default values are 0.1 0.9 0.1 0.9.

GRID	<i>ma mb mc</i>	<p>Change the grid used for calculating the density of atoms in the configuration cell. This grid is used by the commands CPLOT and DPLOT. The grid size is <i>ma</i>×<i>mb</i>×<i>mc</i> (along the a-, b- and c-axis). Default values are <i>ma</i> = <i>mb</i> = <i>mc</i> = 20.</p> <p>NB: <u>If you plot a crystal with CPLOT or DPLOT it is recommended to use values of <i>ma</i>, <i>mb</i>, <i>mc</i> which are multiples (in each direction) of the number of cells building the configuration. If you have a small grid, atoms at different positions within a grid-cell will be treated as having the same position. This may lead to apparent shifts of the positions in the plot.</u></p>
HCDENSITY	<i>hdlow hdhigh</i>	Set density limits <i>hdlow</i> and <i>hdhigh</i> for histograms. This is used to set the borders of the 'contour'-plot created by HCPLOT. If <i>hdlow</i> or <i>hdhigh</i> < 0, the limits will be set automatically.
HCPLOT	[<i>mgn</i>]	Plot a 'contour'-plot of the histogram density, in a plane through the cell. The plane orientation can be changed by CUT, and the 'contour' limits by HCDENSITY. A magnification of the plot can be set by <i>mgn</i> . Default value for <i>mgn</i> = 1.
HDENSITY	<i>hdens</i>	Set surface density <i>hdens</i> for histograms, used by HDPLOT. The region is opaque for histogram density > <i>hdens</i> and transparent for histogram density < <i>hdens</i> . If <i>hdens</i> < 0 the surface density will be set automatically.
HDPLOT		Plot a 3-D surface around a constant histogram density. The surface density can be changed by HDENSITY. A magnification of the plot can be set by <i>mgn</i> . Default value for <i>mgn</i> = 1.
HELP		Write a short list of available commands.
HOPEN		Open a new histogram file for plotting. If no filename is given ConfPlot will ask for the file via a browse window (Window version only).
LEGEND		Toggle legend box ON/OFF. If legend is ON a legend box will be plotted in the case of density and spin dot product plots
LIGHT	[<i>x y z [diffuse shine polish]</i>]	<i>x,y,z</i> determines the direction to the light illuminating the plot. Default values are −1.0 −1.0 −0.5. The other parameters determine the diffusiveness, shininess and polish of the plot. Default values are 0.2 0.8 1.0.

MULTIPLE	<i>nr</i>	It is possible to make multiple plots merged together. By choosing a value of <i>nr</i> , no actual plotting will occur until <i>nr</i> CPLOT/DPLOT/PLOT/SPLOT commands have been issued. <u>DON'T change any colours before all <i>nr</i> commands have finished.</u>
OPEN	[<i>filename</i>]	Open a new configuration file for plotting. If no filename is given ConfPlot will ask for the file via a browse window (Window version only).
PAGE	[<i>width, height</i>]	Sets the <i>width</i> and <i>height</i> of the plot in cm units. Subsequent plots are however scaled to fit in the current plot window if either <i>width</i> or <i>height</i> is larger than the current size. Default values are given by the current size of the physical plot window.
PAUSE		Used in command files to make a pause in the execution of a command file. Execution is resumed by pressing <ENTER>.
PLOT	[<i>mgn</i>]	Make a plot of the configuration with atoms as balls and/or bonds. Colour and radius can be changed with ATOM, RADIUS and SBOND. A magnification of the plot can be set by <i>mgn</i> . Default value for <i>mgn</i> = 1.
POLYGON	<i>itype1 itype2 rmin1 rmax1 rmin2 rmax2</i>	Plot polygon surfaces between atoms of type <i>itype2</i> around atoms of <i>itype1</i> if the distances between the <i>itype1</i> and <i>itype2</i> atoms are greater than <i>rmin1</i> and less than <i>rmax1</i> and if the distances between <i>itype2</i> atoms are greater than <i>rmin1</i> and less than <i>rmax1</i> . Default polygon colour is red.
NOPOLYGON	[<i>itype1 itype2</i>]	Deletes polygons between atoms of type <i>itype2</i> around atoms of type <i>itype1</i> . If no arguments are given then all polygons are deleted.
PRINT	[<i>/prdevice</i>]	Set hardcopy output device to <i>/prdevice</i> , the plot will be written to a file instead of the screen. If no device is given the default will be to write to a postscript file. (The screen is the default device).
RADIUS	<i>itype radius</i>	Set the radius of atoms of type <i>itype</i> to <i>radius</i> . This is used by PLOT. Default radius is 0.4 Å.
RCOLOURS	[<i>ic1 [ic2..]</i>]	Plot RMC curves using coloured lines [<i>ic1 [ic2..]</i>]. Max. no. of plotted/specified lines/colours is 10. Default values are initially black, red, green, ..., green+cyan and then the colours set by the previous call to RCOLOURS.
RCSELECT	[<i>rc1 [rc2..]</i>]	Select which RMC curves to plot. Default are all curves in the current group and plots.

RFIT	[igroup [icurve [rxmin rxmax rymin rymax]]]	Make Gaussian peak fit(s) to the RMC curve <i>icurve</i> in group <i>igroup</i> , plotting $rxmin < x < rxmax$, $rymin < y < rymax$. Default values are the current group and curve (selected by RGSELECT and RCSELECT) and the current plot limits (selected by RPLOT).
RGSELECT	[igroup]	Select which RMC group to plot. Default is the first group.
RLINES	[is1 [is2..]]	Plot RMC curves using styled lines [is1 [is2..]]. Available styles are 1 - , 2 - , 3 - , 4 - and 5 - . Max. no. of plotted/specified lines/styles is 10. Default values are initially 1,...,5 and then the styles set by the previous call to RLINES.
ROPEN		Open a new RMC output file for plotting. If no filename is given ConfPlot will ask for the file via a browse window (Window version only).
<u>RESOLUTION</u>	<i>ires</i>	The size and resolution used by PRINT. Three values are valid <i>ires</i> =1 low-resolution small hardcopy file, <i>ires</i> =2 medium-resolution (default) and <i>ires</i> =3 high-resolution and big hardcopy file (may take very long time).
ROTATE	<i>axis angle</i>	Rotate the configuration <i>angle</i> degrees around the axis <i>axis</i> . Valid values for <i>axis</i> : x y or z.
RPLOT	[rxmin rxmax rymin rymax]	Plot the current RMC curve(s)/plot(s)/group with $rxmin < x < rxmax$, $rymin < y < rymax$. Default values are the data limits $\pm 10\%$.
RPSELECT	[ip1 [ip2..]]	Select which RMC plot(s) in the current group to plot. Default is all plots within the current group.
RTITLE	"title"	Outputs the string "title" as a title above the top axis, used with RPLOT.
NORTITLE		Make the RPLOT title invisible.
RXCAPTION	"xcaption"	Outputs the string "xcaption" as a caption below the bottom axis, used with RPLOT
NORXCAPTION		Make the RPLOT x caption invisible.
RYCAPTION	"ycaption"	Outputs the string "ycaption" as a caption to the left of the left axis, used with RPLOT
NORYCAPTION		Make the RPLOT y caption invisible.
SBOND	[icolour [brad]]	Set the colour of bonds to the colour represented by index <i>icolour</i> (see colour index list) and radius of bonds <i>brad</i> . Default values are red and 0.1 Å.
SCREEN	[/scdevice]	Set output device to screen (default). The screen device used is given by <i>/scdevice</i> , if this is blank the default is windows /W9.
SETCLR	<i>icolour r g b</i>	Set the colour <i>icolour</i> to the red, green and blue values, $0 < r, g, b < 1$.

SHIFT	<i>sfa sfb sfc</i>	Shift atoms in the cell relative to the a-, b- and c-axis. The fractional distances are <i>sfa</i> , <i>sfb</i> and <i>sfc</i> respectively. Limits are $-1 < sfa, sfb, sfc < 1$. Default values are <i>sfa</i> = <i>sfb</i> = <i>sfc</i> = 0 (no shift).
SLICE	<i>width</i>	Make a slice of the configuration <i>width</i> Ångström wide. The slice is centred around a point (<i>aa,bb,cc</i>) and directed orthogonal to the normal (<i>na,nb,nc</i>). Both (<i>aa,bb,cc</i>) and (<i>na,nb,nc</i>) should previously be set by the command CUT. Every new call of CUT - SLICE will cut away more from the configuration. Applies to PLOT and SPLOT commands.
NOSLICE		No slicing, all atoms in the configuration are restored.
SPIN	[<i>filename</i>]	Open spin orientation file (of the same format as the configuration files).
SPLOT	[<i>mgn</i> [<i>stype</i>]]	Plot spin arrows at positions given by the configuration file (opened with OPEN) and in directions given by the spin orientation file (opened with SPIN). A magnification of the plot can be set by <i>mgn</i> . Default value for <i>mgn</i> =1. Two versions of spin plot are possible, <i>stype</i> =0 (default) arrows will have the colour corresponding to the atom colour, <i>stype</i> =1 a continuous colour map will be used and depends on the value of the dot product (see DOTPRODUCT).
SPOLYGON	[<i>icolour</i>]	Set the colour of polygons to the colour represented by index <i>icolour</i> (see colour index list). Default colour is red.
SYMMETRIZE	<i>ispg isett [irec]</i>	Applies the relevant symmetry operations of spacegroup no. <i>ispg</i> in the <i>isett</i> setting to density plots. If the current plot object is in the reciprocal space then the <i>irec</i> flag must be set (any integer will do).
NOSYMMETRY		Do not apply symmetrisation.
TEXT	" <i>text</i> " <i>x y</i>	Outputs the string enclosed by "" at position <i>x y</i> (in fractional frame units)
UNITCELL	<i>n1 n2 n3</i>	To make a sensible density plot of a configuration which is made up of a number of unit cells, it is possible to shift the atoms into one unit cell. Number of cells in configuration along the a, b and c direction are <i>n1</i> , <i>n2</i> and <i>n3</i> . This command can be used before CPLOT and DPLOT.

VIEW	$v_x v_y v_z v_p$	Shift the view of the configuration along the x-, y- and z-axis with v_x , v_y and v_z respectively. $v_x = v_y = v_z = 0.0$ to centre the plot. To shift the configuration left $v_x < 0$, right $v_x > 0$, down $v_y < 0$, up $v_y > 0$, away from you $v_z < 0$ and toward you (in to the configuration) $v_z > 0$. The values of v_x , v_y and v_z are relative to the size of the configuration i.e. 0.5 give half and 1.0 the whole length along the configuration box. The parameter v_p describes the perspective of the configuration box. A large value of $v_p \sim 1000$: give a flat 2-D view (looking from a distance). A small value of $v_p \sim 0$: give a 3-D view (looking from a short distance). Default values are $v_x = v_y = v_z = v_p = 0.0$.
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NB: Any of the commands in the list can be read from a “command file” by typing @**filename** at the prompt (where **filename** is the name of the command file).

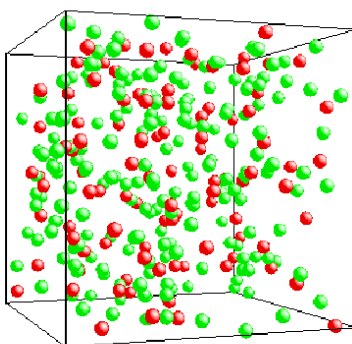
Colour index list:

Index	Colour	Index	Colour
0	Black	8	Orange
1	White	9	Green + Yellow
2	Red	10	Green + Cyan
3	Green	11	Blue + Cyan
4	Blue	12	Blue + Magenta
5	Cyan	13	Red + Magenta
6	Magenta	14	Dark Grey
7	Yellow	15	Light Grey

Example 1.

Read a file containing a configuration of SiO₂.

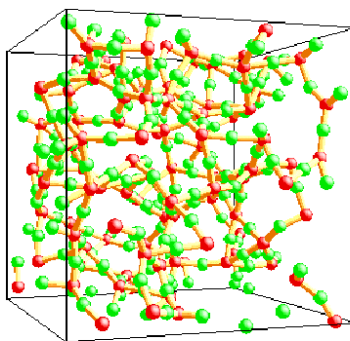
```
> background 1      Set background colour to white (best if you intend to send the picture to a
                    printer).
> box 0             Set box colour to black.
> rotate y 20       Rotate the configuration box 20° around the y-axis.
> plot
```



In this example the colours red (Si) and green (O) is selected automatically from the colour index list.

If we want to add bonds between Si and O which are closer than 2.0 Å from each other type:

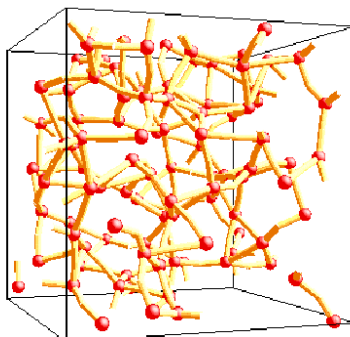
```
> bond 1 2 0.0 2.0  Create bonds between Si (type 1) and O (type 2) where maximum distance
                    between atoms are 2.0 Å.
> sbond 8           Give orange colour to bonds.
> plot
```



If we want to delete the Oxygen from the plot.

```
> noatom 2
> plot
```

Delete atom type 2 (O).



Note that the bonds are still present, to delete them use the command NOBOND.

Example 2.

Read a configuration of ND₄Cl consisting of 12x12x12 unit cells this can be presented as:

```
> unitcell 12 12 12
> background 1
> box 0
> rotate y 20
> radius 1 0.01
> radius 2 0.01
> radius 3 0.01
> plot
```

Merge the 12 x 12 x 12 unit cells into one unit cell.

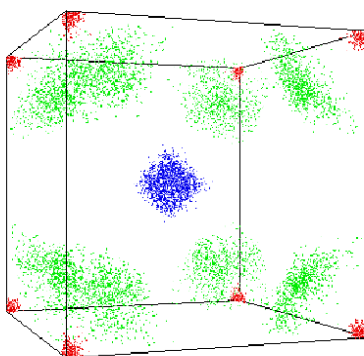
Set background colour to white.

Set box colour to black.

Rotate the box 20° around the y-axis.

Set the atom radius for type 1 to 0.01 Å. (This small radius will plot a point)

Plot it.



```
> cut 0.667 0.667 0.667 1 1 1
```

Cut a plane through the (2/3,2/3,2/3) coordinate of the unit cell

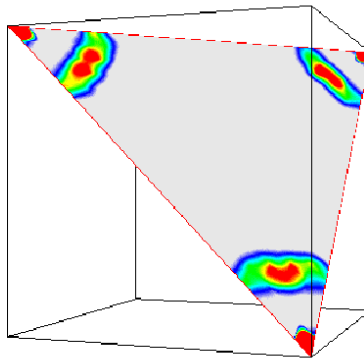
and orientated orthogonal to the (1,1,1) direction.

Look at the cell from a better angle.

```
> rotate y -40
```

> cplot

Make a plane 'contour'-plot.



> rotate x 20
> multiple 2
> cut 0. 0.2 0. 0 1 0

> cplot
> cut 0. 0. 0.5 0 0 1
> cplot

Rotate 20° around the x-axis.

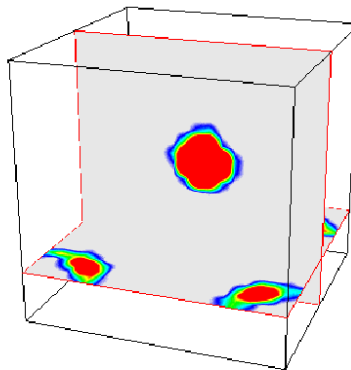
Make two plots in one.

Cut a plane through the (0,0.2,0) coordinate of the unit cell and oriented orthogonal to the (0,1,0) direction.

First subplot of two (nothing will show on the screen).

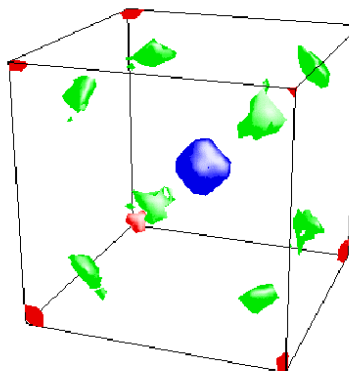
Cut a second plane .

Second and final subplot, now it should plot on the screen.



> dplot

Make a 3-D surface plot.



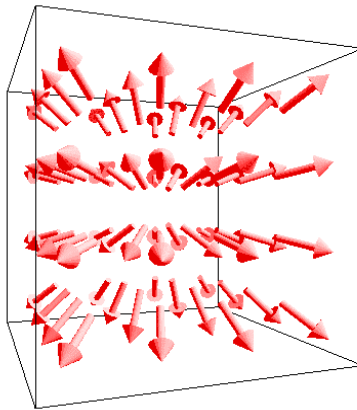
> exit

Example 3.

Read a configuration file containing atom positions *myconf.cfg* and a spin orientation file *mypin.cfg*:

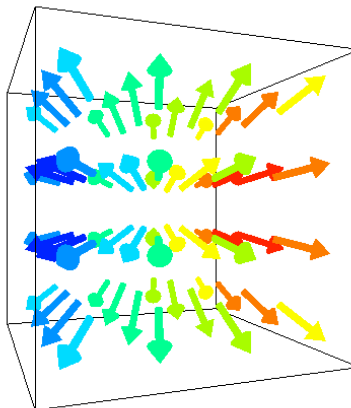
> open myconf.cfg
> spin myspin.cfg
> background 1
> box 0
> rotate y 20
> splot

Open file with atomic positions.
Open file with spin orientations.
Set background colour white.
Set box colour black.
Rotate 20° around the y-axis.
Plot it, all arrows have the same colours as corresponding atom type.



> splot 1 1

Plot colour coded arrows, the colours depends on the dot product between the x-axis (DOTPRODUCT 1 0 0) and the spin direction.

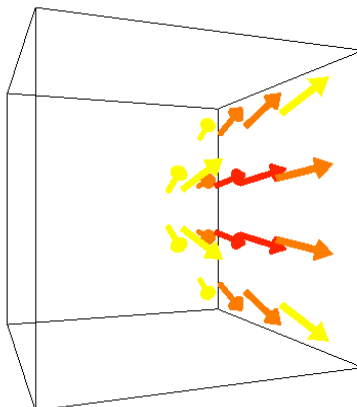


> dotproduct 1 0 0 0.5 1.0

Select arrows with dot product between x-axis and spin direction. Values between 0.5 - 1.0.

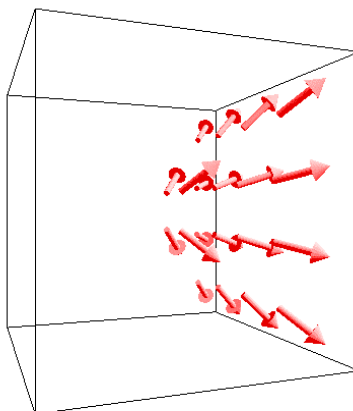
> splot 1 1

Colour coded plotting.



> splot

Atom colours.



> exit

The program can be found on NFL ftp-server through our web page <http://www.studsvik.uu.se> .

Please send you comments about this program to:

Per Zetterström, email: perz@studsvik.uu.se

References

[1] T.J.Pearson, California Institute of Technology, USA. website:
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