

Useful programs connected to RMC

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Introduction

This manual describes a suite of programs that can be used in connection with Reverse Monte Carlo (RMC) modelling. The programs were originally made to work on a VAX/VMS system but they have now been modified to work on a PC/WIN95/NT/XP and PC/LINUX as well. There may be some small differences between the actual runtime appearance and the versions described here, but it should hopefully be obvious how to use them. In the first section a short description of all programs is given divided into sections according to their intended use for atomic and/or magnetic configurations. In the next section we describe the common approach of using symmetry operations for building and analysing crystalline configurations. Finally some of the programs are described in more details. For information about WinNFLP, RMC, MCGR, ConfPlot etc., see the manuals for these programs.

ACKNOWLEDGMENTS

The PGPLOT © [1] and PGXTAL © [2] packages (with some minor modifications) are used for all 2D and 3D graphical output. A number of numerical algorithms from Numerical Recipes [3] are used in modified forms. Following is a (incomplete) list of the persons contributing to the original code used in the various programs:

A. Hannon, M. A. Howe, D. Keen, R.L. McGreevy, A. Mellergård, L. Pusztai, P. Zetterström, A. Wannberg, J. Wicks.

Programs for creating and modifying atomic and magnetic configurations (UsefulCfg)

AddAtom	Adds atoms next to others within an existing network
AddAtomRel	Adds atoms next to others, in specific direction, within an existing network
AddRand	Adds atoms at random positions within an existing network
CoOpt	Atoms are swapped in order to satisfy coordination constraints
Crystal	Produces a crystal configuration from a .ATOM coordinate file, using spacegroup symmetry information
DelAtom	Removes atoms, renames atoms type or split atoms of one type into multiple types. Selection can be made by coordination constraints, from an atom index list file, or as a fraction of or all atoms of a kind
GaussAtoms	A Gaussian distribution of displacements is added to the configuration. Different displacements for each type permitted
MidBond	Creates a configuration of bond midpoints
MidPt	Adds atoms at bond centres
MolToAtoms	Converts a configuration of molecules into one of the constituent atom
MoveOut	Atoms are moved apart in order to satisfy cut-off constraints
MultSize	Programme to alter box size by considering the starting configuration as a unit cell and choose the number of such cells along each edge
MultSizeSpin	Programme analogous to MultSize for spin configurations
Random	Produces a random position configuration
Randomise	Programme to randomise order of particles in array
RandomNumbers	This program creates a file .RAN of random numbers, for use in e.g. DelAtom
RandomSpins	Program to make a random orientation spin configuration
ReSize	Alters the box size by reducing the density, but with same no of atoms
Size	Alters box size by cutting to obtain the desired no of atoms
SpinMagAv	Replaces spins with the average direction within some integration distance
SpinRot	Rotates spin configurations uniformly about some axis
SpinSym	Produces an ordered spin configuration from a .SPIN parameter file
SpinToMol	Convert spins to diatomic molecules
UnitCell	Collapses points into a unit cell (being a subdivision of the configuration cell)

Programs for analysing atomic configurations (UsefulAnalyzeCfg)

AvMove	Compares two configurations and calculates rms movements
BondVal	Calculates bond valence sums for a pair of atom types in a configuration
CfgDiff	Calculates the difference between two configurations
Disp3D	Program to fit 3D Gaussian distributions to displacements from crystal sites
Displace	Calculates rms displacements from crystal sites in specific directions
FindAtoms	Finds atoms at specific crystallographic sites
FreeVol	Calculates free volume of atoms
Gr3D	Calculates a partial 3D g(r) for one or more configurations
GrDir	Calculates the partial g(r)'s and S(Q)'s for one or more configurations along a specific direction or in a specific plane
GrSq	Calculates the partial g(r)'s and S(Q)'s for one or more configurations
GrSq_MOL	Calculates the partial g(r)'s and S(Q)'s for one or more configurations. The molecular version
Grtheta	Calculates the partial g(r,theta) where theta is the angle with respect to the direction of some specific neighbour atom
gsv	Calculates the average g(r) and standard deviation from an .GSV file
Neigh	Distribution of neighbour coordination numbers
NextTo	Calculates number of neighbours of each type
Per	A program to use random walks to calculate resistance
Resistivity	Calculates the "resistivity" of a configuration
Rings	Calculates distribution of 1-x-1-x-1 rings e.g. Si-Si-Si in SiO2
Triplets	Calculates triplet (angle) correlations
Volume	Extract atom numbers from FreeVol output

Programs for analysing magnetic configurations (UsefulAnalyzeScfg)

FindSpins	Finds spins within a specific angle from a crystallographic direction
MuMuR	Calculates differential and integrated $\langle [\mu(0) \mu(r)]^N \rangle$, where N=1,2 or 3, for each partial magnetic type, possibly in a specific direction or plane
MuMuRTh	Calculates the spin-spin ($r_{ij}, \cos(\theta_{ij})$) distribution of spin pairs for each r bin within a specific r interval as well as the mean $\cos(\theta_{ij})$ and $\cos^2(\theta_{ij})$
MuMuXYR	Computes the mux(r) and muy(r) spin correlations as defined by Blech and Averbach [4]
Nematic	Convert spins in triangular clusters to their normals as defined in [5]
SpinCoAng	Calculates the 2D distribution of spin pair cosines, for type A atoms, and A-B-A bond cosines, for type A and intermediate type B atoms within specific neighbour distances
SpinCoDist	Calculates the 2D distribution of spin pair cosines, and average distance to selected neighbours
SpinMap	Calculates the 2D spin polar and azimuthal angle distribution relative a specific axis=z' or x' axis
SpinMod	Calculates distribution of spin modules, useful with for e.g. Nematic and Tetra programs
SpinNeigh	Calculates the spin-spin cos(theta) distribution of spin pairs within a specified r interval as well as the mean cos(th) and cos(th)^2. A file listing atoms with average neighbour spin-spin projection larger than a specific angle can also be produced
SpinTot	Calculates average spin axis and magnitude for each type of magnetic atom. Optionally outputs a list of atoms with spins deviating more than a specified angle from the average axis
Tetra	Convert spins in tetrahedral clusters to their average

Programs for creating and modifying data files (UsefulData)

Add	A programme to add constant values to x and/or y values
Addcol	A programme to add a new column to a DATA file
Average	A programme to calculate the average y value

Convol	A programme to convolute $g(r)$ or $f(Q)$ with a Heaviside function in order to take into account the limited r box size or experimental Q range
ConvRes	A programme to convolute scattering data with a Gaussian resolution function
Coord	Program to calculate coordination number from $g(r)$
Extract	Extract a column from a RMC plot file to a DATA file
FFAdd	Program to add a paramagnetic form factor column to a DATA file
FFSub	Program to subtract a paramagnetic form factor from a DATA file
Flatline	A programme to replace y data with a constant
FormFactors	Program to calculate magnetic or x-ray average squared and partial form factors
FPToDATA	Program to convert FullProf instr=0 or 5 format data to NDP formats
GaussErr	A programme to create a DATA file containing Gaussian distributed errors
Integrate	A programme to integrate a DATA file
Merge	A programme to merge y columns from two DATA files into one file
Multiply	A programme to multiply constant values to x and/or y value
NDPtoRiet	Program to convert NDP F(2theta) formats to Rietveld format. Errors from input file included in output
Partials	Calculates partial scattering coefficients and angles between vectors
Qrange	A programme to select the Q range of a DATA file
QThetaQ	Program to convert DATA format files from $f(2\theta)$ to $f(Q)$ or vice versa
ReduceLog	Code for reducing RMCPOW log files to columns of log values. All text lines except summary coding is stripped.
Remerge	A programme to remerge y columns from one DATA file into two files
Sqav	A programme to get the average $(Q^{*}q_w)^{*}y$ for a DATA file
Stogtos	A programme for transforming $S(Q)$ to $G(r)$ or vice versa
Strip	A programme to strip data file of unwanted columns
Xcoeff	Calculates x-ray form-factors
Yoverx	A programme to calculate $I(Q)/Q$ or $G(r)/r$
Ytimesx	A programme to calculate $I(Q)*Q$ or $G(r)*r$

Programs for plotting data files (UsefulPlot)

c3d	A programme to do a file suitable for 3D ball and stick plots of a configuration
CellDens	Program to calculate the unitcell density 3D histogram for a given atom type with optional symmetrisation.
Fqplot	Used to plot corrected structure factors from default-files *.fq or any other extension, with GENIE, TEXT or DATA format.
Preplot	Used to plot *.pre files from Prep1. A and B positions of the instrument are plotted separate.
Prevplot	Used to plot *.pre files from Prep1 normalised to a Vanadium standard .pre-file. UP, MIDDLE and DOWN banks for the A and B positions are plotted both separate and merged.
RasMolConv	Program to convert RMC configurations to format suitable for RASMOL
RMCFit	A simple peakfit program for data from RMC or USEFUL output files or data with GENIE, TEXT or DATA format
RMCPlot	This program plots output files from RMC and various USEFUL programs
SpinD2	A programme to do a file suitable for 3D plots of a spin configuration
SqPlot	Used to plot UP, MIDDLE and DOWN data files created by Prep2
XYPlot	General XY plotter for DATA files using PGPLOT

From unit cells to configurations

The basic entity for building a crystalline model is the unit cell. The metrics of this cell is given by the cell edge and angle parameters or, equivalently, it's three basis vectors. The unit cell may be primitive or centred. In addition to simply building configurations as multiples along each basis vectors we can use a generalised approach where in principle any parallelepiped, containing the same periodicity as the primitive cell, can be used as building blocks for the model. For this purpose we define an intermediate cell (IC) being a supercell of the primitive cell but not necessarily the conventional unit cell. The whole configuration is then constructed as multiples of IC:s in the traditional way. Transformation matrices

conveniently describe relations between the various cells used and we give below the definitions used. Spacegroups are given according to the numbering in IT and the setting also follows the order in IT. Cell edges [\AA], a_1 - a_3 and angles [$^\circ$], g_1 - g_3 are to be given for the IT conventional cell.

'Intermediate' cell (IC) generation:

$\text{isym} > 0 \rightarrow$ the IT conventional unit cell (UC) is used as IC
 $\text{isym} = 1 \rightarrow$ Primitive cell
 $\text{isym} = 2 \rightarrow$ A centred cell
 $\text{isym} = 3 \rightarrow$ B centred cell
 $\text{isym} = 4 \rightarrow$ C centred cell
 $\text{isym} = 5 \rightarrow$ I centred cell
 $\text{isym} = 6 \rightarrow$ F centred cell
 $\text{isym} = 7 \rightarrow$ Rhombohedral cell in hexagonal setting
 $\text{isym} = 8 \rightarrow$ Hexagonal primitive cell
 $\text{isym} < 0 \rightarrow$ A non-standard IC is generated from the corresponding UC by a transformation matrix P^{UI}

The transformation matrix $P^{UI} = (p_{ij})$ is defined by the relations between the two sets of basis vectors \mathbf{a}_i and \mathbf{A}_i , where $i=1,2,3$, for the UC and IC respectively according to

$$\mathbf{A}_i = p_{1i}\mathbf{a}_1 + p_{2i}\mathbf{a}_2 + p_{3i}\mathbf{a}_3 \quad (2)$$

For computational purposes a common least denominator is taken out of the matrix and given separately. E.g., to convert a UC to its C-centred supercell we can take

$$\mathbf{A}_1 = \mathbf{a}_1 + \mathbf{a}_2, \quad \mathbf{A}_2 = -\mathbf{a}_1 + \mathbf{a}_2, \quad \mathbf{A}_3 = \mathbf{a}_3 \quad (3)$$

so that the common denominator is 1 and the transformation matrix is

$$P^{UI} = \begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (4)$$

i.e. $(\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3) = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3) P^{UI}$. The same formalism can of course also be used to construct an IC smaller than the UC. E.g. to construct the rhombohedral primitive cell of a face centred cell we instead use

$$\mathbf{A}_1 = \frac{1}{2}(\mathbf{a}_1 + \mathbf{a}_2), \quad \mathbf{A}_2 = \frac{1}{2}(\mathbf{a}_2 + \mathbf{a}_3), \quad \mathbf{A}_3 = \frac{1}{2}(\mathbf{a}_3 + \mathbf{a}_1) \quad (5)$$

so the denominator is 2 and

$$P^{UI} = \begin{pmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix} \quad (6)$$

For visualisation of a configuration it must be related to a Cartesian coordinate system. Also, spin calculations are easier with Cartesian coordinates. Various RMC and USEFUL programs use the following definitions: ($\hat{\mathbf{A}}_i$ and \mathbf{x}_i are unit vectors of the IC basis and Cartesian systems resp.)

$\text{icart} = 1 \rightarrow \hat{\mathbf{A}}_1 = \mathbf{x}_1, \hat{\mathbf{A}}_2 \perp \mathbf{x}_3, \hat{\mathbf{A}}_{22}, \hat{\mathbf{A}}_{33} > 0$, default for $\text{isym}=1$ to 6
 $\text{icart} = 2 \rightarrow \hat{\mathbf{A}}_2 = \mathbf{x}_1, \hat{\mathbf{A}}_3 \perp \mathbf{x}_3, \hat{\mathbf{A}}_{23}, \hat{\mathbf{A}}_{31} > 0$
 $\text{icart} = 3 \rightarrow \hat{\mathbf{A}}_3 = \mathbf{x}_1, \hat{\mathbf{A}}_1 \perp \mathbf{x}_3, \hat{\mathbf{A}}_{21}, \hat{\mathbf{A}}_{32} > 0$
 $\text{icart} = 4 \rightarrow \hat{\mathbf{A}}_1 = \mathbf{x}_1, \hat{\mathbf{A}}_3 \perp \mathbf{x}_2, \hat{\mathbf{A}}_{22}, \hat{\mathbf{A}}_{33} > 0$, default for $\text{isym}=7$ to 8
 $\text{icart} = 5 \rightarrow \hat{\mathbf{A}}_2 = \mathbf{x}_1, \hat{\mathbf{A}}_1 \perp \mathbf{x}_2, \hat{\mathbf{A}}_{23}, \hat{\mathbf{A}}_{31} > 0$
 $\text{icart} = 6 \rightarrow \hat{\mathbf{A}}_3 = \mathbf{x}_1, \hat{\mathbf{A}}_2 \perp \mathbf{x}_2, \hat{\mathbf{A}}_{21}, \hat{\mathbf{A}}_{32} > 0$

Input and output

For ease of use with complex systems many programs can be run in a semi-interactive mode where relevant input data are read from parameter files whereas names of output files usually are given interactively. Saving the parameter files also helps to log how a configuration was created, analysed or changed. These files are generally assumed to have the default extension .par although any other extension is possible. The structure of the various input files is given below together with the program descriptions. A collection of template files is also included in the USEFUL package. However, for simpler cases, with not so many parameters, programs can in most cases also be run fully interactive (which might also give a clue to why an input file is not working). Another common feature of many of the programs is the ability to conveniently handle the averaging and error estimation of results based on multiple configurations. In this context a **set** is a group of configurations collected with the same simulation conditions, e.g. fitted to the same experimental data at some particular temperature. Different sets could then e.g. correspond to simulations using data at a series of temperatures.

Environment variables

There are a number of environment variables that need to be defined in order to run some of the NFL programs. If the USEFUL programs are run under the WinNFLP program the default values are read from the file NFLP_logicals.ini residing in the same directory as the WinNFLP executable. Some of the variables can be modified using the FILES: OPTIONS menu item. Optionally the new values can be saved. If you are using WinNFLP over a network (see above) a local copy of this file is saved to the directory that WinNFLP is started in. If you are using LINUX or VMS these environment variables need to be defined in e.g. your login file. Following is a list with examples of the syntax used for Windows. Note that all variables that are directories must end with a \ (/ in LINUX and] in VMS).

NDP_FORMAT = TEXT

The file format for NDP data files (used by PREP1, CORRECT etc.), can be GENIE, DATA or TEXT.

SLAD_CAL_CUR = C:\Anders\SLAD\Cal\Mar01.prm

SLAD instrument calibration file.

SLAD_RAW = \\R2exp1\SLAD1\

Location of SLAD raw data files.

NXSECTION = c:\NFLP\Tables\nxsection.dat

Neutron nuclear scattering cross-sections table.

MXSECTION = c:\NFLP\Tables\mxsection.dat

Neutron magnetic scattering cross-sections table.

XXSECTION = c:\NFLP\Tables\xxsection.dat

X-ray scattering cross-sections table.

DOUBLESCATTERING = c:\NFLP\Tables\doublescattering.dat

A table for multiple scattering corrections used by CORRECT.

NFLP_TABLES = c:\NFLP\Tables\

Location of tables (such as the ones above) used by NFL programs.

NFLP_TEMPLATES = c:\NFLP\Templates\

Location of template forms for input files used by NFL programs.

NFLP_DOCUMENTATION = c:\NFLP\Documentation\

Location of help documents for NFL programs.

PGPLOT_FONT = c:\NFLP\Tables\grfont.dat

File containing fonts used by PGPLOT applications

PGPLOT_DEV = /W9

Default screen output device for PGPLOT applications

EDIT= C:\WINNT\SYSTEM32\notepad.exe

Your favorite text editor. Used to open files with the items in the EDIT menu of WinNFLP

USER_PROGRAMS = c:\NFLP\UserPrograms\

Location of user written programs. These can then be accessed from the USEFUL: USER menu item.

Programs for creating and modifying atomic and magnetic configurations (UsefulCfg)

ADDATOM

Adds atoms close to other atoms in a configuration defined by coordination of the target atoms.

Example If you have a configuration of atom types X and Y, add atom type Z at a distance of 1 Å from each X atom that has 6 Y atoms as neighbours:

```
Input configuration      : xy.cfg
Maximum bond lengths    : 0.0 3.5 0.0          X-X X-Y Y-Y bond lengths
Coordination of targets [From,To,Number]: 1 2 6 Atom type 1(X), 2(Y), with
coordination number 6
Distance away from target atom: 1.0           1 Å from the X atom
Type of atom to place: 3                     Add atom type 3(Z)
Maximum no. to place: 900
No. of atoms added = 500
Config. size           = 1500

Add more atoms (T/F): F
Output file: xyz.cfg
```

ADDATOM REL

Adds atoms at positions, defined by (x,y,z) coordinates, relative to a chosen type of atoms in a configuration.

ADDRAND

Adds a number of atoms randomly (without any constraints) to a configuration.

CRYSTAL

Creates a crystal configuration of atoms that can be used as input to RMC. Input can be read from a file or given manually. Optionally, random Gaussian or correlated harmonic displacements can be added to the equilibrium positions.

Example of manual input create 5x5x5 cells of AgBr:

```
Atom data input file [.atom] :                ! Manual input
Apply to existing configuration [t/f] > f      ! Make a new configuration
Space group and setting > 225 1              ! F m-3m spacegroup
Reading symmetry data from
C:\Anders\Prog\NFLProg\Tables\spacegroups.dat
UC lattice parameters > 5.74 5.74 5.74 90. 90. 90. ! Cell edges and
angles
isym and no of cells in each direction> 6 5 5 5 ! F centered, 5x5x5 unit cells
Displacement type [n/p/g] > n                ! No displacements
No of atomic types > 2                      ! Two atom types, Ag and Br
nW > 1                                       ! No of Ag Wyckoff sites
Wyckoff site and x,y,z > 4a 0 0 0
nW > 1                                       ! No of Br Wyckoff sites
Wyckoff site and x,y,z > 4b .5 .5 .5
Output in RMC coordinates [t/f] > t
No of generated/displaced atoms
    1 500
    2 500
Total no of generated atoms is 1000
Output file [.cfg] > AgBr
```

Example of input file create 6x4x6 cells of LaMnO3 with harmonic displacements added:

```
.false.                ! cfgexist
62 1                   ! ispg, isett
5.732361 7.666631 5.530905 90.0 90.0 90.0 ! a1,a2,a3,g1,g2,g3
1 6 4 6               ! isym,n1,n2,n3
p                     ! disptype
```

```

300. 200. 17. 2   1      ! TDLONG, TDTrans, Tabs, imod, idisp
3                      ! No of atom types
      1 138.0          ! No of La Wyckoff sites,Mmol
4c 0.04850  0.25000 -0.00807 ! Wyckoff site,x,y,z
      1  55.0          ! No of Mn Wyckoff sites,Mmol
4b 0.00000  0.00000  0.50000 ! Wyckoff site,x,y,z
      2  16.0          ! No of O Wyckoff sites,Mmol
4c 0.48735  0.25000  0.07394 ! Wyckoff site,x,y,z
8d 0.30557  0.03852  0.72448 ! Wyckoff site,x,y,z
.true.          ! RMC coordinates used in output
lamno3.cfg

```

-end of input file-

This example generates a 6×4×6 Pnma LaMnO₃ configuration with a Debye model (imod=2, if imod=1 a modified sinusoidal Debye model is used) of harmonic displacements, given by the atomic masses Mmol (amu), longitudinal and transversal Debye temperatures TDLONG and TDTrans and absolute temperature Tabs (K)

cfgexist: If this is false a new configurations is created else random or correlated displacements can be added to an existing configuration (the filename must then be given on a new line immediately after cfgexist)

Spacegroup selection, ispg and isett, is described above

Cell edges [Å], a1-a3 and angles [°], g1-g3 are to be given for the conventional cell.

'Intermediate' cell (IC) generation is described above. For isym < 0 a non-standard IC is generated from the corresponding UC by reading (from additional lines following isym,n1,n2,n3) the UC to IC tranformation matrix, a common denominator and a code for Cartesian coordinate systems) (also describe above)

Configuration cell generation: n1,n2,n3 is the no of IC's along each IC basis vector

Displacements generation: disptype =

- n → no displacements
- p → harmonic displacements
- g → random displacements with Gaussian distribution

For disptype = n, idisp =

- 1 → Mmol [amu] is read and the mean square displacement u2 is determined
- 2 → u2 (Å²) is read instead of Mmol and an 'effective' mmol is determined

For disptype = g, u2 (Å²) is always read

Output coordinate units:

- RMC - standard RMC configuration coordinates, -1<x,y,z<1
- CC - configuration cell coordinates, 0<x,y,z<1

If the final item, the output filename, is left blank or skipped then the filename is asked for at runtime

DELATOM

Either deletes atoms or changes their type. The atoms are selected by index numbers (produced by e.g. RANDOMNUMBERS) or coordination of the target atom.

MIDPT

Places atoms at the mid-point of bonds between atoms in a configuration.

MOVEOUT

Move atoms in a configuration apart if they are too close together.

Example In a configuration of X and Y type atoms, move them apart so that all distances are greater than 1.5Å (do it in steps with increasing distances):

```

Starting configuration (no extension) ? xy
(version 3 format configuration file)
Output file           : xymov
Closest approaches   : 1. 1. 1.           Closest approach between X-X
X-Y Y-Y
88 atoms of type 1 have too close neighbours
106 atoms of type 2 have too close neighbours
Move atoms of type 1 ? (T/F) : T
Move atoms of type 2 ? (T/F) : T
Maximum move         : 0.05
Max. no. of iterations : 50000
.
.
.
0 atoms of type 1 have too close neighbours after 3526 iterations
0 atoms of type 1 have too close neighbours after 5417 iterations
Re-calculate neighbours? (T/F) : F
Change cut-offs ? (T/F)       : T
Closest approaches           : 1.5 1.5 1.5           New closest approach
.
.
.
0 atoms of type 1 have too close neighbours
0 atoms of type 2 have too close neighbours
Re-calculate neighbours? (T/F) : F
Change cut-offs ? (T/F)       : F

```

RANDOM

Creates a random configuration of atoms that can be used as input to RMC (without any constraints on closest approach). You select number of atoms and number density of the system.

RANDOMNUMBERS

Creates a file of random numbers within specified limits. This list of numbers can be used to delete or substitute randomly selected atoms in a configuration (use DELATOM).

SIZE

Changes the size of a configuration.

UNITCELL

To get a better understanding of RMC results from crystalline samples, it may be useful to shift the atoms in all unit cells into one merged cell. This new single unit cell configuration contains all the points representing the atoms. This merged configuration should be used as input to the program CELDENS2A. A good idea is to give the output file the extension `.cel` to avoid confusions with the original configuration file.

Programs for analyzing atomic configurations (UsefulAnalyzeCfg)

GRSQ

Calculates $G(r)$ and $S(Q)$ from a configuration file.

NEIGH

Calculate the number of neighbours within defined distances in a configuration. The result is written to a text file.

TRIPLETS

Calculates triplet correlations, i.e. angle or cosine distribution between three atoms in a configuration file.

Example Calculate the angle distributions for the AgBr configuration created by CRYSTAL in the example above (use only atoms closer than 5.0 Å from each other):

```

No. of theta pts           > 180
No. of neighbours for bond ang (0 for all) > 0
Number of configurations    > 1

```



```

Configuration file          > agbr.cfg
Maximum r values           > 5.0 5.0 5.0
Output file                > agbr.trp
(A)ngle or (C)osine distribution [C] > A

```

Programs for creating and modifying data files (UsefulData)

CONVOL

Convolutes a structure factor with a step function corresponding to half the box length $L/2$ of a configuration. A measured structure factor comes from a sample with “infinite” size, the configuration in a RMC calculation has a limited size. It is thus necessary to use the convoluted structure factor in RMC calculations.

COORD

Calculates the coordination numbers over peaks in $g(r)$.

EXTRACT

Extract data sets from a multiple set file. EXTRACT can be used on .OUT files produced by RMC or MCGR.

PARTIALS

Calculates (neutron) scattering coefficients that are needed in RMC, MCGR and GRSQ.

Example Calculate the coefficients for heavy water:

```

No. of atom types           : 2
Relative concentrations      : 2 1
No. of data sets           : 1
No. of differences          : 0
(Difference coefficients to come in pairs
after single data set coefficients)
Atom symbols/scattering lengths for data set 1 : D O
Give scattering lengths or atomic symbols:

6.671000E-01
5.803000E-01
Name for output files       : d2o

```

The output file d2o.par should look like:

Coefficients:

```

Data set 1
  1.977878E-01    1.720525E-01          D-D    D-O
  3.741646E-02          O-O    Used by RMC

Sum of coefficients:  4.072568E-01          Used by MCGR

```

Normalised coefficients:

```

Data set 1
  4.856586E-01    4.224670E-01
  9.187438E-02

```

Angles between vectors :

.00

Cosines between vectors :

1.00

StoGtoS

Calculates $g(r)$ from $S(Q)$, or $S(Q)$ from $g(r)$ by Fourier transformation.

Programs for plotting data files (UsefulPlot)

CELLDENS

Divides a configuration (usually a merged configuration produced by UNITCELL) into a number of resolution elements (parallelepipeds). The number of atoms (density) of a specified type in each element is calculated, and written to a file. This file can then be used by some graphical software (like IRIS Explorer) to plot the probability of atoms occupying different regions of the configuration. This program can be run with an input file.

Example Use the configuration `xy.cel` produced by UNITCELL. The configuration contains atom types X and Y, we are interested in the density of X:

Type of atom > **1** X atom

Number of resolution elements (x,y,z) > **20 20 10**

Here the cell is divided into 20x20x10 parallelepipeds, use a number proportional to the configuration edges.

Number of input files > **1**

Input file > **xy.cel**

Offset vector > **0 0 0** Usually 0 0 0

Symmetrise (t/f) > **f** Some simple symmetrisation can be applied.

Output file > **file.x**

RMCPLOT

A program to make quick plots of data sets from a multiple set file. It can be used to plot .OUT files produced by RMC or MCGR and various output files from USEFUL programs.

[1] PGPLOT Copyright © 1983-2001 by the California Institute of Technology.

<http://astro.caltech.edu/~tjp/>

[2] PGXTAL Copyright © D. S. Sivia, 1997. PGXTAL. <http://www.isis.rl.ac.uk/dataanalysis/dsplot/>

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