RSpace Users Manual

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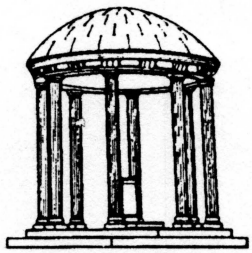

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RSpace

A reciprocal-space modelling tool

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RSspace - A Reciprocal-Space modelling program.

M R Harris Sept '87
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Introduction

Rspace is an interactive program designed to help crystallographers plan data-collection strategies when using diffractometers equipped with area detectors.
It provides a graphical representation of Ewald's construction in which the crystal frame can be rotated, depicting the volume of reciprocal space that has been swept by the projection of the area detector on Ewald's sphere.
The program allows the user to enter experiment-specific parameters, and then specify collection scans by jumping to a chosen crystal orientation and interactively rotating about a goniometer axis. The volume of reciprocal space swept by the scan is then displayed graphically, superimposed on various structures representing the goniometer, the asymmetric volume of reciprocal space, the laboratory and the crystal axes. Gaps and redundant collections in the strategy can be identified as the simulated collection proceeds. Scanned regions may optionally be mapped to symmetry-equivalent positions; this allows depiction of a contiguous scanned volume when data is collected in regions of reciprocal space that are actually distant from each other, but which have symmetry equivalents that are adjacent.
Both rectangular and circular detectors can be modelled, for use with the Xuong-Hamlin, Xentronics and FAST systems, amongst others.
Broad-spectrum Laue diffraction can also be modelled.
The current version is a C-language program that runs under UNIX or VMS on Masscomp or VAX processors, driving Evans and Sutherland ps300 displays. There are also options to write out a polygon file readable by the UNC Pixel-Planes graphics engine, or to supress all graphical output.

Starting the program

The program is invoked with the command 'rspace', with the following optional parameters :

'-d device_name' specifies the device for graphics output. Possibilities are:

'ps300' (by far the wisest choice)
'm0' or 'm1' (Masscomps - under development)
'Pixel-Planes_file' (only useful at UNC)
'Null_device' (supresses graphical output)

'-i setup_file' specifies a file of initial commands to execute. If not specified, a file called 'rspace.init' is sought in the current directory, and if found, commands are read from that. These files can be created with an editor, entering the commands just as if you were answering the interactive prompts. Comments can be flagged by a '#' or a '!' in the first column.

'-s' supresses searching for rspace.init.

'-y' or '-n' respectively cause and inhibit a fresh download of the ps300 networks. The default is to be prompted.

'--' or '-h' print a reminder of the command-line options, then exit.

Alternatively, the program can be invoked with VMS-like options, for example:
$ rspace /d=ps300 /i=rspace.script /n /s
Note that there must be spaces between the options.

Issuing commands

Keyboard entries comprise single letter commands optionally followed by parameters; prompts are issued if no parameters are given on the command line, and the defaults that will be used if carriage-return is hit are indicated. If insufficient parameters are given on the command line, or if the parameters are not interpretable, the remaining fields are filled with the default values, with the exception of the 'jump' command, which requires all three parameters to be specified.

To avoid problems when reading from scripts, it was decided not to reprompt on error, so commands should be re-entered if an error message suggests that you response was not acceptible.

Although only the initial letter is needed, the commands are referred to in the documentation by one-word mnemonics beginning with the appropriate character; it is recommended that these mnemonics are used in command scripts.

Most commands have lower-case initials, the exceptions being rarely-used. Typing 'help' or '?' at any prompt will give helpful information and reprompt. At the "RSpace <> :" and "Setup <> :" prompts, a particular help topic may be specified, either as a parameter, or at the "help <> :" prompt. Typing 'quit' at any prompt will abort the current operation. n The commands are divided into those which require a major rebuild of the image structures, and those which simpy manipulate the structures; the former are only accesible through the 'Setup' command, which removes previous scans.

The structure of unsolicited messages from the program is loosely based on the VMS approach, with fields as follows : An initial question-mark is followed by the name of the originating routine, a severity code, and an explanation of the condition that caused the message to be sent. Possible severity codes are s,i,w,e,f and a. (success, informational, warning, error, fatal and apology), e.g. ?check_limits-e-Omega axis out of bounds. Warnings indicate that something unusual has happened, but as long as the user knows what he is doing, execution can continue happily. Errors indicate that the user has done something wrong, and that the path of execution has changed because of it. Fatal errors are so hideous that continued execution would be futile or misleading. The program will often commit suicide because them.

An example session

Invoke the program with the command 'rspace -d ps300'. Answer 'yes' to the download question, and wait for the "RSpace <> : " prompt, at which point you should see some structures on the PS300; try to orient yourself. Type 'setup', then at the "Setup <> : " prompt, type 'ask'. You will then be asked a series of questions about your crystal and detector system. If you need more explanation about a prompt type 'help', and if you want the default values presented in angle brackets, hit carriage return.

Once RSpace has enough information, it will draw representations of the real and reciprocal cell axes, the laboratory axes, and the area detector, along with a sphere encompassing data within your chosen resolution limit. You will then be asked about the orientation of the unique volume of data that you want to have displayed. Except for the triclinic and monoclinic groups, you will choose one of a selection of volumes, but for the higher-symmetry groups you may also add some arbitary rotations.

Then you will be returned to the "RSpace <> : " prompt, and a series of collections can be made using the command 'jump' to get to the starting position, and 'omega', 'chi' or 'phi' to perform the scan. You can also move the detector from this prompt.

If you wish to change a small number of Setup parameters, you can enter Setup and type the particular commands you want, instead of using 'ask'.

'exit' will return you to the main prompt, leaving other values unchanged, with the exception of the unique-volume orientation, for which it will prompt. When you are satisfied that your strategy covers the required volume, 'follow_path' will display the trajectory you followed, allowing you to examine the complete strategy. 'write_to_file' will save your parameters in a file that can be read in at a subsequent RSpace session, or saved to allow you to enter the values into the real diffractometer- driving program.

Geometry

In Ewald's construct, the active collection area is defined by the projection of the area detector from the centre of Ewald's sphere to its surface. For a square detector, this patch is dish-shaped with curved edges, a most inconienient shape to display with vector graphics. For this reason we represent the patch as a flat surface with the same shape as the original detector, with the edges of the patch touching Ewald's sphere. This results in the corners being a little too far out, and the centre a little too far in. If this discrepancy becomes bigger than about 10% of Ewald's radius, we draw radiating lines from the true centre of the detector to its rim, but still don't round the edges. The resulting pyramid allows the true curved surface to be easily visualised. Not rounding the edges seems reasonable, since the detectors that can move in close enough to have significant curvature are likely to be circular and thus have no protuding corners.
If a range of wavelengths has been specified, the projections corresponding to the two extremes are drawn, with corners joined to form a box.

Coordinate systems

All coordinate systems are right handed. The laboratory axes are centred on the crystal, with the positive x axis running along the X-ray beam from the crystal away from the source, the positive y axis pointing towards the ceiling, and the z axis in the horizontal plane. The conventional real and reciprocal crystal axes, a,b,c and a*,b*,c* are used.
The goniometer axes are as follows : Looking from the top of the goniometer with the omega motor at the bottom, a positive omega rotation is anticlockwise. At chi = 0, the phi motor is at the bottom of the chi circle, and a positive phi rotation is clockwise. Looking from the beam source towards the crystal, with omega = 0, a positive chi rotation is clockwise. If your system is not like this, the sense of rotation about each axis can be reversed using the command 'sense_of_rotation'.
If your phi motor is opposite the omega motor when chi = 0, you should change the value of PHI_START in rspace.h to -1.0 and recompile.
For the detector position, a positive angle corresponds to an anticlockwise rotation when viewed from above.

PS300 specifics

Under VMS, the PS300 device to be used can be specified by defining the logical name PSDEVICE to be a suitable string, as defined in the PAttach section of the PS300 manual. This string is of the form :
"logdevnam=device_name/phydevtyp=interface_type", including the quotes.
If the logical name is not defined, or you are running under UNIX, the default device specified at compile time in the header file will be used. If you did not specified download on the command-line, you will be prompted :
'Download networks (y/n) ?'; yes and no respectively cause and inhibit a fresh download of the ps300 networks. Networks from previous runs can be used, but remnants of previous runs will flash up briefly before they are overwritten.

It is recommended that a separate terminal is used to issue commands to the host, but the terminal emulator can be used if you don't mind shifting modes from keyboard to function keys often.

The bottom row of dials manipulate the entire structure in screen space. It can be rotated, scaled and clipped at the front and back ('slabbing'). When a jump has been selected, 3 of the top-row dials control goniometer movements, as an alternative to typing in the new angles. For a scan, only the appropriate one of these dials is activated.

The function keys are activated by hitting <shift><line/local>, and the terminal emulator is returned with <line/local>. Switching modes like this is tedious, and it is recommended that a separate terminal is used to invoke the program.
'reset' resets screen-space orientation.

'stereo' gives frame-sequential stereo. This is designed to work with the Tektronics full-screen plates and Millenium active spectacles, on PS300, 330, and 350 displays, but has only been tested on the PS330 with Tektronics plate. Optical-interface spots are displayed in the bottom right-hand corner for machines that use them.
'lateral' gives lateral stereo pairs, if stereo is already on.
'tip' - tips the screen Y axis forward 30 deg. I think this looks nicer. The rest toggle display of the various structures on their labels. When hit with the shift key, function keys 1 through 5 toggle the display of the first 5 scans. Subsequent scans cannot currently be individually toggled.

Laboratory axes are represented as solid lines, crystal axes as short dashed lines, and reciprocal axes as long dashed lines with muted colours. The x, a and a* axes are blue, the y, b and b* axes are red, and the z, c and c* axes are green. The goniometer is represented as a gold-coloured structure comprising a chi circle mounted on a stub representing the omega motor, and carrying a line segment representing the capillary tube. In addition, 3 dim pink axes are drawn along the omega, chi and phi rotation axes. The sphere of resolution is drawn in red, and the unique volume of data in blue.
The detector is initially blue, but changes colour with each scan. Each scanned volume is drawn in the colour of the last static detector. When the goniometer is being interactively positioned with mapping enabled, both the mapped and unmapped detectors are displayed. The unmapped one is bright white, the mapped one a dim green. Mapped and unmapped lab axes are also displayed during interaction.
Until your first invocation of 'setup', a representation of Ewald's sphere is drawn in mauve, tangential to the detector.

The full command set

setup
- ask_for_parameters
- group_number
- dimensions_of_cell
- zone_angles
- type_of_detector
- move_detector
- resolution
- volume_mapping
- keep_lab_axes_fixed
- limits_change
- sense_of_rotation
- Wavelength
- Unique_volume_position
- exit_from_setup

omega
chi
phi
jump_to_position
move_detector
resolution_change
undo_last_move

information_on_current_state
follow_path
write_parameter_file
yank_input_stream_from_file

help topic
new_features
System_command
Doze
quit

'setup' allows access to commands which require a rebuild of major data structures, viz :

:

group_number
dimensions_of_cell
zone_angles
type_of_detector
move_detector
resolution
volume_mapping
keep_lab_axes_fixed
limits_change
sense_of_rotation
Wavelength
Unique_volume_position
exit_from_setup

:

move_detector and resolution can also be invoked from the top-level prompt.

:

When you have entered setup mode, you can either set parameters with the individual commands listed above, or invoke 'ask' mode, which will then prompt you for all the required parameters.

If you choose 'ask' mode, the dialogue will pause at some point, as the program busies itself collating the information that you have given it, in order to display your configuration on the screen. You will then be asked to choose your unique-volume orientation based on the current parameters.

If you choose to change parameters individually, you must indicate completion with the command 'exit' when you have made all the changes you desire. If you did not specify the unique-volume orientation explicitly, you will be prompted for this after the other information has been collated.

On exit, all information about previous scans is lost.

If you choose to quit at the setup prompt, changes you have made during the current setup session will not be undone, but nor will they be incorporated into the graphics display. It is not a recommended manoeuver unless you have just entered setup. Remember that you can save and restore parameter sets with the 'write' and 'yank' commands. Quitting at a subcommand within setup is quite safe, and will not change the parameters for which you were being prompted.

'ask_for_parameters'

starts a dialogue under setup, prompting for all the required parameters. It exits setup mode automatically when completed or if a quit is encountered. Quitting early allows you to skip the later questions if you know that you are going to want the defaults.

'group_number'

allows you to specify the space-group number to define symmetry.

If you do not know your space-group number and enter 0, or if the program does not recognise your response, you will be prompted for the Laue-group number. If you do not know that, consider whether crystallography is really the career for you.

'dimensions_of_crystal'

sets the cell parameters, for use in constructing the crystal axes. Any units may be used for the cell edge lengths, since they are scaled, but angles should be in degrees.

'zone_angles'
sets the zone angles, and the orientation of the crystal.
The zone angles are the set of omega, chi and phi goniometer rotations at which the crystal axes line up with laboratory axes, and thus account for the arbitary orientation of crystals in their capillaries. At the zone, individually-mounted examples of a particular crystal form will be aligned identically.
As well as the three angles, it is also neccesary to specify which crystal axes and planes should align with which laboratory axes and planes. A numbered menu of options is presented to facilitate this. When setup is exited, the program automatically executes a 'jump' to zone.

'type_of_detector'
changes the shape, dimensions and number of the detectors, allowing for both square Xuong-Hamlin detectors and circular Xentronix ones. The program was written for Xuong-Hamlin type detectors, as collection strategies are more complex than for Xentronix types, but differently shaped detectors are easily incorporated.
We support Xentronics detectors simply by changing the shape of the detector, and do not account for the fact that some of these systems have fixed chi angles. To use the program with these systems, you must currently specify the fixed chi angle for each 'jump' and 'zone' command. Setting the upper and lower mechanical limits on chi to 1 degree either side of the fixed value will help prevent mistakes.
Up to two detectors may be specified, but their spatial relationship will be fixed, and they will be mapped as a single unit, based on the position of the centre of the second detector.
Although the detectors should be represented as projections on to a sphere, RSpace takes the liberty of assuming that they are planar. The discrepancy is small.

'move_detector'
moves the detector to a new angle and distance. It can be invoked from within setup, or during a scan sequence. The angle is specified in degrees, with positive angles corresponding to an anticlockwise rotation when viewed from above. The distance is measured from the crystal to the centre of the detector, in millimeters.

'resolution_change'
draws a sphere of resolution at an appropriate radius. This is only a visual guide, and is not currently used in any calculations.

'volume_mapping'
selects or deselects unique-volume and freidel mapping for subsequent scans.
For practical reasons, such as mechanical limits on the movement of the goniometer, it is sometimes impossible to collect a complete dataset in a contiguous region of reciprocal space, and collections from symmetry- equivalent positions have to be made. To address the difficulty in judging how such non-contiguous volumes complement each other, the program can optionally map all swept volumes to equivalent regions of a single unique volume. When mapping is enabled, attempts to scan outside the unique region are pushed into it, according to appropriate symmetry rules. The unmapped scan is also drawn, the mapped version being dimmer.
When interacive positioning has been chosen, a mapped detector will be created according to the mapping function appropriate to the starting position. Note that this mapping may not be appropriate once you have moved the detector.
The simplest mapping scheme is 'all_bijvoits', which maps all scans into a single unique volume that is displayed on the screen. 'freidel' mapping maps the scans into one displayed hemisphere, and 'bijvoits' mapping maps the scans into one of two displayed volumes - the specified one and its Freidel mate, related by inversion symmetry.

The mapping of the whole detector is based on the position of the centre of the detector at 10 intermediate points between each drawn position, so part of the detector may appear outside the chosen volume when near the boundaries. For two-detector configurations, the mapping of both detectors is based on the position of the centre of the second detector. This is fine if the second detector is being used for simultaneous collection of Freidel pairs, but is a limitation under other circumstances. To simulate two independent detectors, you must currently ask for one, perform the scans, and then repeat them with the detector moved to the new position.

The symmetry rules for the mapping operations have been determined for all the protein space groups, but not all have been tested. In particular, there are pairs of space groups that belong to the same laue group, but whose unique volumes align with different axes. There is a mechanism to compensate for this, but it has only been invoked for groups 151/152 and 153/154.

If you know of other such groups (probably in the 140-150 region), please let us know.

The mapping functions are complex, and are difficult to test fully, so please check their behaviour on simple cases when first used on new space groups.

The default is no mapping.

'keep_lab_or_crystal_fixed'

determines which frame of reference stays still during a scan. Fixed lab. axes make the most sense, but because of our implementation, manipulations are a bit squirrely.

The default is laboratory axes fixed.

'limits_change'

sets the mechanical limits of the machine in terms of lower and upper bounds on omega, chi and phi.

'Unique_volume_position'

allows blind positioning of the depicted unique volume.

The unique volume is the asymmetric unit of reciprocal space, and thus includes the minimum amount of data required for a complete collection.

For most space groups there is a finite number of these volumes, since they must be aligned with major crystal axes, but for triclinic and monoclinic groups there are an infinite number because of rotational degrees of freedom. Triclinic groups have two degrees of freedom, and monoclinics have one. Specifying a unique-volume orientation requires a unique-volume number representing one of a finite number of tesellating volumes defined by RSpace, and one arbitary rotation for monoclinic groups, or two arbitary rotations for triclinic groups.

The command is primarily intended for use in scripts, using values determined interactively as setup mode is exited. The unique volume is depicted graphically, and also used by the mapping functions.

'Wavelength'

specifies the radiation wavelength. It prompts for a range, so that Laue diffraction can be modelled. Specifying two identical values gives a monochromatic source.

'sense_of_rotation'

changes the direction of rotation about the goniometer axes.

Three integers specify the direction for omega, chi and phi. +1 gives the rotation senses defined above under 'coordinate systems', -1 reverses the direction. You should use this command if your system does not correspond to the definitions above.

'omega'

performs an incremental scan about the omega axis.

'chi'

performs an incremental scan about the chi axis.

'phi'

performs an incremental scan about the phi axis.

'jump_to_position'
jumps to position, without sweeping a volume.
Successive jumps replace each other, so there is no need to 'undo' them. The word 'zone' can be used as a substitute for the triplet of numbers representing the zone angles.

'undo'
undoes the last jump or increment; successive calls work backwards.
Sometimes this command leaves stains. Sorry.

'yank_input_stream_from_file'
starts reading input from a file.
These files can be created with an editor, entering the commands just as if you were answering the interactive prompts. Comments are flagged by a '#' or a '!' in the first column. Command is returned to the keyboard at the end of the file.

'write_to_file'
writes out a file readable by 'yank'.
It prompts for whether to write just setup parameters, just scan information, or both.
A file of setup parameters can be used as a setup file, and if renamed to 'rspace.init', will be read at each subsequent invocation of RSpace, allowing site-specific or user-specific information to be setup automatically.
A file with setup parameters and scan information can be used to reconstruct complete sessions, or to record final results for entry into the real goniometer-driving program.

'information_listing'
list the current parameter values on the screen.

'follow_path'
shows how you got to your current position.

'help topic'
gives help on any topic at the 'RSpace' and 'setup' prompts, 'help' gives help on the current activity at any prompt.
If more than one page of help is presented, you will be prompted to continue or quit ('c or q') after each screenfull.

'new_features'
types out the latest release notes.

'Doze'
hibernates the program for a few seconds.
The command is useful in scripts for demos and dodgy ethernet links. An optional parameter specifies the number of seconds.

'Pause'
pauses the program until continuation is requested from the keyboard.
A 'quit' will terminate a script if that is where the Pause was issued.

'System_command'
submits a command to the operating system, returning when it is completed.

'quit'
aborts the current activity, but note that quitting from setup mode cannot restore parameters that were changed. Use 'write' to save a state.

'exit'
kills the program after confirmation if issued at the top-level prompt, or returns to the top-level prompt if issued from setup mode, rebuilding major datastructures as it goes. The setup exit takes the optional parameter 'noclear', causing the old scans to be left visible, but still erasing information about how they were created.

'EOF' (<ctrl>D under UNIX, <ctrl>Z under VMS)
from the keyboard causes immediate exit from the program at any prompt.

Known bugs

1) 'Undo' leaves droppings. These are cleaned up on subsequent scans, but are irritating none the less.

2) 'Keep_lab_fixed' behaves a bit squirrely.

3) The goniostat representation loses its outer ring when the resolution limit is set below 2 Angstroms or above 4 Angstroms. *Unknown bugs*

None.