RSAP - A Code for Display of Neutron Cross Section Data and SAMMY Fit Results

February 2001

R. O. SAYER

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Computational Physics and Engineering Division

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RSAP – A Code for Display of Neutron Cross Section Data and SAMMY Fit Results

R. O. Sayer

1. Overview

RSAP is a computer code for display of neutron cross section data and selected SAMMY output. SAMMY [1] is a multilevel R-matrix code for fitting neutron time-of-flight cross-section data using Bayes' method. RSAP, which runs on the Digital Unix Alpha platform, reads ORELA Data Files (ODF) created by SAMMY and uses graphics routines from the PLPLOT [2] package. In addition, RSAP can read data and/or computed values from ASCII files with a format specified by the user.

Plot output may be displayed in an X window, sent to a postscript file (rsap.ps), or sent to a color postscript file (rsap.psc). Thirteen plot types are supported, allowing the user to display cross section data, transmission data, errors, theory, "Bayes" fits, and residuals in various combinations. In this document the designations "theory" and "Bayes" refer to the initial and final theoretical cross sections, respectively, as evaluated by SAMMY. Special plot types include Bayes/Data, Theory - Data, and Bayes - Data. Output from two SAMMY runs may be compared by plotting the ratios Theory2/Theory1 and Bayes2/Bayes1 or by plotting the differences (Theory2 - Theory1) and (Bayes2 - Bayes1).

The term "plot" is used to denote a graphical representation of a combination of data, theory, errors, and Bayes from one ODF file. Several plots may be stacked in a single frame in a window (or page) with a common x-axis. RSAP also supports multiple frames in a window with each frame containing a separate plot. Up to 8 plots may be superposed, or overlaid, in one window with a separate normalization factor applied to each data set. The term "data set" denotes the numerical values of data, theory, etc. in one ODF file.

Data may be plotted as histograms, points, small circles, or large circles. Theoretical values may be displayed as solid or dashed lines. Each axis may be linear or logarithmic. Any one of the colors red, blue, green, cyan, yellow, magenta, or white may be specified for data, theory, Bayes, axes, and text. For example, the specifier:

col y r g

indicates colors yellow for theory, red for Bayes, and green for data. These are the defaults. Note that white ("w") shows well on the screen and in postscript plots, but white is invisible in color postscript plots. A detailed example is presented in section 4.5.

Plots may be annotated in several ways:

- values of resonance energies and widths read from a user-specified "PAR" file.
- user-specified X- and Y-axis label strings.
- User-specified annotation strings may be written at user-specified locations.
- A title string may be written above the plot.

Two text fonts, Simple and Roman, are supported. The default Simple font draws faster on the screen, and the Roman font is more readable for hard copy and publication quality plots.

RSAP produces an ASCII file "**rsap.parcom**" containing a formatted comparison of the user-specified PAR file with the file "SAMMY.PAR" and an ASCII file "**rsap.ratexpth**" in which energies, data, errors, theory, results of a SAMMY Bayes run, and percentage differences are listed. If SAMMY.LPT exists, the final value of the conventional CHISQ/N will be written on the plot.

RSAP reads input from either the keyboard or a file, and produces plots as specified by input quantities. To run RSAP on a DEC Alpha machine in the ORNL CAD farm:

rsap

or

rsap < inputfile

where "**inputfile**" is the name of your input file. Sample RSAP input files are listed and explained in section 4, Example Input Files. Each example corresponds to one of the sample plots displayed in Figures 1-10.

The following sections include discussion of RSAP usage, plot types, RSAP specifiers, example input files, peak search and fitting, and automatic spin group variation.

2. Use of RSAP

This section provides a brief introduction to some of the features of RSAP as well as descriptions of input data files and output plot file formats. More detail is given in sections 3-6.

2.1. Getting Started

A good place to begin is [Example 1](#), which plots data, errors, and the Bayes fit in one frame. Read the documentation in section 4 and run this simple case. Then copy the input file to your directory, and try different options, types of plots, etc. Try one of your ODF files. Run example 2 to stack two frames in one window and example 3 to plot from two ODF files. All example cases may be run sequentially with the script:

/home/ros/axp/RSAP/v5/EXAMPLE/doexamples

Typing "**h**" at the RSAP prompt will list plot types and specifiers.

2.2. ODF Files

RSAP reads ORELA Data Files (ODF) created by SAMMY runs on Digital Unix Alpha workstations. A maximum of 60000 data points is allowed. Data points may be averaged before plotting by using the **avg** specifier.

All ODF files in the user's current directory may be opened by following the **odf** specifier with a space and asterisk e.g., "**odf ***".

SAMMY writes ODF files with energies in units of eV (keV) if the maximum energy is less (greater) than 1 keV. The ODF file structure does not include information on energy units. Thus, the user must specify the energy units, either by the default (keV), or by selecting eV with the specifier "**ev 2**".

2.3. DAT Files

RSAP can read data and/or computed values from an ASCII "DAT" file with a user-specified format. Five quantities are read per record: x, y1, err1, y2, and y3. These quantities can be any set of numerical data; however, in order to use the same RSAP commands as those used for ODF files, the code makes the correspondences $x \Leftrightarrow \text{energy}$, $y1 \Leftrightarrow \text{data}$, $\text{err1} \Leftrightarrow \text{error}$, $y2 \Leftrightarrow \text{theory}$, and $y3 \Leftrightarrow \text{Bayes}$. Note that the initial and final theoretical cross sections evaluated by SAMMY are denoted by the terms "theory" and "Bayes", respectively. Thus the RSAP plot request "**1 dt**" will plot y1 (data) and y2 (theory) vs. x (energy). The user may specify axes labels pertaining to the actual information in the DAT file; for example

```
xlb time
ylb pressure and temperature
```

The default format is (**5e11**), corresponding to the **csirs** data format. Other formats are selected with the **fmt** specifier; for example **fmt (5e20.6)**. A maximum of 60000 data records is allowed. Data points may be averaged before plotting by using the **avg** specifier.

2.4. Multiple Plots in a Window

Multiple plots in a window may be accomplished by specifying more than 1 frame in either the x- or the y-direction through the "**ops**" command. Each frame will contain a plot with unique x- and y-axes. For example, use "**ops 2 3**" to plot 6 data sets in a 2 x 3 matrix in x and y.

Two to eight plots may be "stacked" in the same frame using a common x-axis. A given plot may include any combination of data, theory, and Bayes values. Examples 2 and 3 illustrate the use of the "**ops 1 1 2**" command to stack 2 plots in one frame (see Figures 2 and 3). To plot 8 data sets, stacking 4 plots per frame in a 2 x 1 matrix in x and y:

2.5. Overlay of 2 or more Plots

RSAP allows up to 8 "plots" to be overlaid in the same frame using common x- and y-axes. A particular plot may include any combination of data, theory, and Bayes values. A normalization factor may be applied to each data set via the "**nrm**" specifier as defined in section 3. This overlay feature is most useful for showing general features of fits to several data sets. Example 9 illustrates the use of normalization factors in an overlay.

2.6. Plot File Formats

The color (monochrome) postscript file **rsap.psc** (**rsap.ps**) produced by RSAP may be converted to GIF, JPEG, or TIFF format with the **xv** program. For example, the command

```
xv -rot 90 -cmap rsap.psc
```

displays both **rsap.psc** and the xv control window. Click on "SAVE" in the control window and choose the file format in the "SAVE" window.

RSAP also produces a PLPLOT metafile, **rsap.meta**, that may be rendered with the **plrender** procedure described in Appendix D. For example, to make a color postscript file, **rsap_port**, in portrait orientation:

```
plrender -dev psc -o rsap_port -ori 3 rsap.meta
```

3. RSAP Specifiers and Plot Requests

RSAP input consists of "specifier" cards and plot request cards. At least one "**odf**" or "**dat**" specifier is required to define an input file. Other specifiers such as "**ops**" may be included to set various input parameters. A device specifier (**x**, **ps**, or **psc**) is required to set the output device to (X-window, postscript file, or color postscript file).

Note that the device specifier "**x**" sends the plot to an X plot window, the color postscript file **rsap.psc**, the monochrome postscript file **rsap.ps**, and the PLPLOT metafile **rsap.meta**. Specifiers **ps** and **psc** send output to postscript files only.

After a device specifier, RSAP expects one or more plot request cards. Plot request input consists of the ODF file number, plot type, emin, emax, ymin, ymax in (a2, a4, 4f10) format. X- and Y-axis limits are denoted by (emin, emax) and (ymin, ymax), respectively. Axes limits default to the data limits. RSAP plot types and specifiers are listed in Tables 1 and 2, respectively.

Table 1. RSAP Plot Types

TYPE	DESCRIPTION
1 d	CROSS SECTION Data from ODF file 1
2 d	CROSS SECTION Data from ODF file 2
1 de	Data, Errors
1 dt	Data, Theory (INITIAL theoretical cross section)
1 db	Data, Bayes (FINAL theoretical cross section)
1 det	Data, Errors, Theory
1 deb	Data, Errors, Bayes
1 rt	Residuals, Theory
1 rb	Residuals, Bayes
1 bod	Bayes/Data
1 dtb	Data, Theory, Bayes
1 etb	Data, Errors, Theory, Bayes
1 tmd	Theory - Data
1 bmd	Bayes - Data
a d	TRANSMISSION Data from ODF file 1
b d	TRANSMISSION Data from ODF file 2
a de	TRANSMISSION Data, Errors
a dt	Data, Theory
...	...
12tot	(Theory from file 2) / (Theory from file 1)
12bob	(Bayes from file 2) / (Bayes from file 1)
12tmt	Theory2 - Theory1
12bmb	Bayes2 - Bayes1

Table 2. RSAP Specifiers and Arguments

SPECIFIER	ARGUMENTS	FORMAT	DESCRIPTION example
ann	kpl, ka, kacol ann_string	i1, i1, i2 a40	Plot # for this string 1,2,3 for left, center, right above frame top 4,5,6 for left, center, right below frame top color annotation string ann 14 This is an annotation
avg	kaverage	i2	# of data points to average before plotting avg 12
bug	kdebug	i2	> 0 says print debug information
cap	capt_string	a64	Caption string - up to 64 characters cap This is a caption
cmf	cmf_name	a72	Command file name - up to 72 characters
col	kt,kb,kd,ka,kt	5a2	colors for theory,Bayes,data,axes,text one of "y","r","g","c","b","m","w" col y r b
dat	dat_name	a72	DAT file name - up to 72 characters dat /home/xyz/u235/mydata
ev	kplev	i2	= 2 says ODF energies are in eV > 0 says resonance energies, widths in eV ev 2
fmt	fmt_string	a72	format string for dat files fmt (5e20.4)
fnt	kfont	i2	1 (2) says SIMPLE (ROMAN) font fnt 2
h			prints "help" messages
lab	kodf, kdate, kchi	3i2	= 0 : don't write odf name, date, chisq/n lab 0 0 0
log	kx, ky	2i2	kx (ky) > 0 says logarithmic x (y) axis log 0 1
lpr			sends rsap.ps to default printer
nrm	Anorm(1-8)	8f	Normalize ODF File i by Anorm(i) nrm 1.0,2.4,0.76,8.25
odf	Odfname *	a72 a1	ODF file name - up to 72 characters Reads up to 8 ODF files in current directory odf /home/xyz/u235/total.odf
ops	nx,ny,kstack, kpts, keres,kgamr	6i2	# x frames, # y frames, # plots stacked, 0=histogram, 1=dots, 20(21)=small(big) circles > 0 says write res. Energies, Widths ops 1 1 2 1 1 1
ovr	kover	i2	Overlay kover plots in 1 window (kover < 9) ovr 2
exp	exp_string	a72	String for plot request specifier Default: exp 1 dtb

Table 2, RSAP Specifiers and Arguments, cont.

SPECIFIER	ARGUMENTS	FORMAT	DESCRIPTION example
par	inparfile	a72	PAR file name - up to 72 characters par my_par_file_name
pks	fwhm, bias, a2targ, ltarg, Jtot, gamgam, fwhmax	7f	see section on Peak Search and Fitting pks 1.1,3.0, 235.,0.,0.5,0.5,1.2
q			tells RSAP to quit.
rat	kratout	i2	> 0 says write values to file "rsap.ratexpth"
sam			run SAMMY using PAR file <u>rsap.peaks</u>
sgi	sgi_name	a72	SAMMY input file name - up to 72 characters sgi my_SAMMY_input_file_name
sgd	sgd_name	a72	SAMMY data file name - up to 72 characters sgd my_SAMMY_data_file_name
sgr	numres, jsg1, ..., jsg8	9i4	SGV resonance number, spin group list sgr 25, 4, 5, 6
sgv	esglo, esghi	2f8	min and max energies for SGV fit sgv 380.,430.
sgp			Automatic plot of SGV fit results
sym	ksymodf(1-8)	8i4	ksymodf(i) = symbol for ODF file i sym 1,20,21,0,22
sys	command	a72	execute Unix "command" sys mv oldname newname
tit	title_string	a32	32-character title string tit my_plot title
txt	kt, ktc,ol, xt,yt, sizet, angle, txtstring	2i4, 4f8.1, a40	Od# #, text color, position (xt, yt), size, angle, 40-character text string txt 1,9,250.3,200.,2.0,,MyText
xl	xaxlabel	a24	24-character X-axis label xl my X-axis label
yl	yaxlabel	a24	24-character Y-axis label yl my Y-axis label
x			output to X-window, rsap.ps, rsap.psc, rsap.meta
ps psc			output to file rsap.ps output to file rsap.psc
###			Comment - ignored by RSAP

4. Example Input Files

Ten sample RSAP input files are described in this section. Each example corresponds to one of the sample plots displayed in Figures 1-10. The specifier "### " introduces a comment line that is ignored by RSAP.

Note that the device specifier "x" sends the plot to four devices: an X plot window, a PLPLOT metafile **rsap.meta**, the color postscript file **rsap.psc**, and the monochrome postscript file **rsap.ps**. The postscript files may then be sent to the default printer:

"lpr -h rsap.ps" or "lpr -h rsap.psc".

A postscript file may be viewed via **"ghostview -seascape rsap.psc"**.

A postscript file may be created without plotting to an X window by replacing the specifier "x" with "ps" or "psc".

Example 1. One Plot in One Window

This input compares **JohnFowl235_990203.par** and the final SAMMY parameter file **SAMMY.PAR**, reads **JohnFowl235_990203.odf**, and plots one frame (nxp=nyp=1) to an X window. The **"deb"** card specifies a plot of cross section data with error bars and the Bayes fit for $2200 < E < 2500$ keV with y-axis limits of 0 and 1.0 b. If axis limits are not specified, the plot will span the range of data values. Resonance energies and widths are displayed (keres=1, kgamres=1) on the plot. A blank card ends the input for this particular plot sequence and causes the plot to be drawn on the output device. The "q" in column 1 tells RSAP to quit. The "###" comment card is ignored by the code.

```
par /home/ros/axp/RSAP/v5/EXAMPLE/1/JohnFowl235_990203.par      (a4,a72)
odf /home/ros/axp/RSAP/v5/EXAMPLE/1/JohnFowl235_990203.odf      (a4,a72)
tit JohnFowl235_990203 3.784                                     (a4,a32)
### ops: nxp=1,nyp=1, kstack=0, kpoints=1,keres=1,kgamres=1
ops 1 1 0 1 1 1                                                (a4,6i2)
x          output device      (x , ps, psc)
1 deb 2200.,2500.,0.0,1.00                                       (a2,a4,4f10)
```

q

To make the above plot on your X terminal, type:

```
rsap < /home/ros/axp/RSAP/v5/EXAMPLE/1/inx
```

You should see a plot like the one in [Figure 1](#). On your screen the background should be black. After RSAP reads the **"deb"** card and sends the plot to your screen, the code waits for a "RETURN" before reading the next input card.

Alternately, the "x" and "1 deb" cards could be replaced by one **"oxp"** card:

```
oxp 1 deb 2200.,2500.,0.0,1.00                                  (a4,a2,a4,4f10)
```

Figure 1. `/home/ros/axp/RSAP/v5/EXAMPLE/1/inx`

The "par", "tit", and "ops" specifiers are optional. The default "ops" values are:

<code>nxp=nyp=1</code>	(1 plot in x direction, 1 plot in y direction),
<code>kstack=1</code>	(1 plot per frame),
<code>kpoints=0</code>	(plot data as histograms),
<code>keres=kgamres=0</code>	(no display of resonance energies, widths).

Above the plot the ODF file name, title, date, and time are listed. If the SAMMY output file SAMMY.LPT exists, the conventional CHISQ/NDAT is also listed above the plot. If `keres=1`, spin group numbers are listed just above the bottom x axis, and resonance energies are listed just below the top x axis. Resonance energies greater than the x-axis maximum are listed to the right of the plot.

To see an example of stacking 2 plots in a window ([Figure 2](#)) , type:

The upper plot in Figure 2 shows both the residuals (dots) and the Bayes fit.

Example 3. Plot from 2 ODF files

Plots from two ODF files may be stacked in one window:

```
par /home/ros/axp/RSAP/v5/EXAMPLE/3/o16/990203/JohnFowl235_990203.par
odf /home/ros/axp/RSAP/v5/EXAMPLE/3/o16/990203/JohnFowl235_990203.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/3/o16/990203/duanesh_990203.odf
tit 990203. JohnFowl235 + duanesh
### ops: nxp=1,nyp=1, kstack=2, kpoints=0,keres=1,kgamres=1
ops 1 1 2 0 1 1 (a4, 6i2)
x
1 deb 2250.,2450.,0.0,0.80 (i2,a3, 4f10)
2 dtb 2250.,2450.,0.0,1.5
```

To make the above plot on your X terminal (see [Figure 3](#)) , type:

```
rsap < /home/ros/axp/RSAP/v5/EXAMPLE/3/inxs2
```

Note that the code will terminate properly when the end of the input file is reached.

Figure 3. `/home/ros/axp/RSAP/v5/EXAMPLE/3/inxs2`

Example 4. Transmission plots

Transmission data may be displayed by plot requests that begin with "a" or "b" instead of "1" or "2" as shown in the following sample input which contains two plot sequences. In the first sequence, transmission ("a det 0.,400.,0.0,1.0") and total cross section data ("1 det 0.,400.") from the first ODF file are stacked in one frame in an X plot window (see Fig. 4A). The second sequence produces a similar plot (Fig. 4B) for the second ODF file. Note that the "lpr" specifier automatically sends the monochrome postscript file **rsap.ps** to the default printer.

```
odf /home/ros/axp/RSAP/v5/EXAMPLE/4/bal27orthin_990309.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/4/bal27orthick_990309.odf
tit Al27 ORELA thin,thick. AV 5 Title a32
avg 5
col r g b
ops 1 1 2 1 0 0
x
a det 0.,400.,0.0,1.0
1 det 0.,400.,0.,40.

lpr
x
b det 0.,400.,0.0,1.0
2 det 0.,400.,0.,40.

lpr
q
```

To make the above plots on your X terminal (see [Figures 4a, 4b](#)) , type:

```
rsap < /home/ros/axp/RSAP/v5/EXAMPLE/4/alortrantot
```

In this example the plot contains the text "< 5>" at the top of the frame, indicating that 5 data points were averaged before plotting.

Figure 4A. /home/ros/axp/RSAP/v5/EXAMPLE/4/alortrantot

Figure 4B. /home/ros/axp/RSAP/v5/EXAMPLE/4/alortrantot

Example 5. Colors, Fonts, and Annotation

Colors, fonts, and annotation with a character string are illustrated by the following input file:

```
ev 2
avg 2
log 0 1
odf /home/ros/axp/RSAP/v5/EXAMPLE/5/233b10trn.odf
ops 1 1 1 0 0 0
tit "col y r g" (DEFAULT COLORS)
col y r g
x
1 etb 250.0,270.0,10.,200.

### switch to Roman font for postscript output
fnt 2
psc
1 etb 250.0,270.0,10.,200.

### rename color postscript file to "rsapyrg.psc"
sys mv rsap.psc rsapyrg.psc
tit "col b m c - blue, magenta, cyan"
### blue, magenta, cyan for theory, Bayes, data"
col b m c
### switch back to Simple font for screen
fnt 1
### put annotation at location 5 (center)
ann 5 Annotation_string
x
1 etb 250.0,270.0,10.,200.

### switch to Roman font for postscript output
fnt 2
psc
1 etb 250.0,270.0,10.,200.

sys mv rsap.psc rsapbmc.psc
q
```

To make the above plots on your X terminal (see [Figure 5](#)) , type:

```
rsap < /home/ros/axp/RSAP/v5/EXAMPLE/5/incolxpsc
```

Figure 5. /home/ros/axp/RSAP/v5/EXAMPLE/5/incolxpse

Example 6. Figure Captions using "cap"

A 64-character figure caption string may be written at the bottom edge of the plot window with the **cap** specifier. Vertical axes are scaled to fit plots and caption in the window. An example is given in Figure 6, which was produced by the file :

```
/home/ros/axp/RSAP/v5/EXAMPLE/6/incap
```

```
par /home/ros/axp/RSAP/v5/EXAMPLE/1/JohnFowl235_990203.par
odf /home/ros/axp/RSAP/v5/EXAMPLE/2/bcjav3ndsh_990203.odf
ops 1 1 0 1 1 0
cap Figure 6. /home/ros/axp/RSAP/v5/EXAMPLE/6/incap
fnt 2
x
1 dtb 4100.,4700.,0.5,3.5
q
```

Figure captions are supported for the case of one plot per page in the x-direction, i.e. $n_{xp} = 1$ (**ops** 1).

Figure 6. /home/ros/axp/RSAP/v5/EXAMPLE/6/incap

Example 7. Plotting from 3 ODF Files and Annotation Strings

Plotting from 3 ODF files and annotation strings are illustrated in [Figure 7](#), which was produced by the command:

```
rsap < /home/ros/axp/RSAP/v5/EXAMPLE/7/in3odf

par /home/ros/axp/RSAP/v5/EXAMPLE/7/JohnFowl235_990203.par
odf /home/ros/axp/RSAP/v5/EXAMPLE/7/JohnFowl235_990203.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/7/duanesh_990203.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/7/FJF73lows6_990824.odf
tit Plot from 3 odf files
### odf#, pos, col, txtstring      (a4, i1, i1, i2, a40)
ann 14  PLOT 1 JohnFowl235. Position 4
ann 25  PLOT 2 duanesh. Position 5.
ann 36  PLOT 3 FJF73lows6. Position 6
###  nxp,nyp, kstack, kpoints,keres,kgamres

ops  1 1 3 1 0 0
x
1 etb 2250.,2450.,0.0,0.80
2 etb 2250.,2450.,0.0,1.5
3 det 2250.,2450.,0.0,1.5

q
```

The **ann** specifier can be used to position a text string at the left (4), center (5), or right (6) of the plot.

Figure 7. `/home/ros/axp/RSAP/v5/EXAMPLE/7/in3odf`

Example 8. Place 6 Plots in 1 Window

To put plots from 6 ODF files in a single window in a 2x3 xy matrix and send the file `rsap.ps` to the default printer:

```
rsap < /home/ros/axp/RSAP/v5/EXAMPLE/8/inpl_231

par /home/ros/axp/RSAP/v5/EXAMPLE/8/FJF73lows6_991005.par
odf /home/ros/axp/RSAP/v5/EXAMPLE/8/DROTnob_991005.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/8/bBH_aftercj_991005.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/8/bcjav3ndsh_afterBH_991005.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/8/FJF73lows6_991005.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/8/JohnFowl235_991005.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/8/duanesh_991005.odf
tit Plot from 6 odf files
###      odf#, pos, col, txtstring          (a4, i1, i1, i2, a40)
ann 15   PLOT 1 DROTnob_991005 POS 5
ann 25   PLOT 2 JohnFowl235_991005 POS 5.
ann 35   PLOT 3 bBH_aftercj_991005 POS 5.
ann 45   PLOT 4 FJF73lows6_991005 POS 5
ann 55   PLOT 5 bcjav3ndsh_afterBH_991005 POS 5
ann 65   PLOT 6 duanesh_991005 POS 5
ops 2 3 1 1 0 0
x
1 etb 3200.,4000.
5 etb 2250.,2450.,0.0,0.80
2 etb 3200.,4000.
4 etb 2250.,2450.,0.0,1.5
3 det 3200.,4000.
6 det 2250.,2450.,0.0,1.5

lpr
q
```

Other sample input files in the `EXAMPLE/8` directory will plot in a 3x2 xy matrix (`in6odf_321`), and in a 6x1 xy matrix (`in6odf_stack6`).

Figure 8. `/home/ros/osp/RSAP/v5/EXAMPLE/8/inpl_231`

Example 9. Overlay 6 Plots in 1 Window

The number of plots to be overlaid is determined by the **ovr** specifier. To overlay plots from 6 ODF files in a window (see [Figure 9](#)) :

```
rsap < /home/ros/axp/RSAP/v5/EXAMPLE/9/inovr6

par /home/ros/axp/RSAP/v5/EXAMPLE/8/FJF73lows6_991005.par
odf /home/ros/axp/RSAP/v5/EXAMPLE/8/DROTnob_991005.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/8/bBH_aftercj_991005.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/8/bcjav3ndsh_afterBH_991005.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/8/FJF73lows6_991005.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/8/JohnFowl235_991005.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/8/duanesh_991005.odf
tit RSAP v.5. OVERLAY 6 odf files
### omit odf name, write date, omit CHISQ/N
lab 0 1 0
ylb Cross Section in barns
ovr 6
### Normalization factors for odf files 1 - 6.
nrm 1.0,1.0,3.0,0.2,10.,1.
log 0 1
### Roman Font
fnt 2
ops 1 1 1 1 0 0
x
1 etb 0000.,6300.,0.02,20.
2 etb 3200.,4000.
3 det 3200.,4000.
4 etb 2250.,2450.
5 etb 2250.,2450.
6 det 2250.,2450.

q
```

Normalization factors were applied to each plot with the **nrm** specifier, and the **lab** specifier was used to inhibit output of the odf name and CHISQ/NDAT to the plot.

Figure 9. `/home/ros/axp/RSAP/v5/EXAMPLE/9/inovr6`

Example 10. Text Strings using “txt”

Text strings may be written at user (x,y) locations with the `txt` specifier. String size, orientation, and color may be specified as illustrated in Figure 10, which was produced by the file :

```
/home/ros/axp/RSAP/v5/EXAMPLE/10/intxt

ev  2
odf /home/ros/axp/RSAP/v5/EXAMPLE/5/233b10trn.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/5/233b10trn.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/5/233b10trn.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/5/233b10trn.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/5/233b10trn.odf
odf /home/ros/axp/RSAP/v5/EXAMPLE/5/233b10trn.odf
ops 2 1 3 1
tit text string test
lab
### Roman font
fnt 2
### red yellow green blue cyan magenta white
### 1 2 3 9 11 13 15
###
### nodf,col, xt, yt, sizet, angle, string (2i4, 4f8, a40)
txt 1, 9, 250.3, 200., 2.0, ,Double Size-----20-----30
txt 2, 3, 250.5, 220., 1.0, ,Normal Size-----20-----30-----40
txt 3, 1, 251., 200., 0.5, ,Half Size-----20-----30-----40
txt 4,13, 250.5, 200., 1.0,-45.,****TEXT STRING AT -45 DEGREES****
txt 5,13, 250.4, 20., 1.1, 45.,****TEXT STRING AT 45 DEGREES****
txt 6,13, 251., 10., 0.9, 90.,****TEXT AT 90 DEGREES****
x
1 db 250.0,255.,0.0,250.
2 db 250.0,255.,0.0,250.
3 db 250.0,255.,0.0,250.
4 db 250.0,255.,0.0,250.
5 db 250.0,255.,0.0,250.
6 db 250.0,255.,0.0,250.

sys mv rsap.psc rsaptxt.psc
q
```

Figure 10. /home/ros/axp/RSAP/v5/EXAMPLE/10/intxt

5. Peak Search and Fitting

A peak search procedure has been implemented in RSAP to provide an initial PAR file for use with SAMMY. The procedure, an adaptation of the method of Mariscotti [3], is based on computation of the second derivative of the data averaged over a width parameter, **fwhm**. A second parameter, **bias**, is approximately the number of standard deviations above background for a peak to be found. A peak search is requested with the "**pks**" specifier.

```
pks fwhm, bias, a2targ, Itarg, Jtot, gamgam, fwhmax (a4,7f10)
```

where **fwhm** is the full width at half-maximum (FWHM) in eV, **bias** is the sensitivity parameter, **a2targ** is the mass number of the target, **Itarg** is the target spin (I), **Jtot** is the total spin (J), **gamgam** is the capture width in eV (default 1.0), and **fwhmax** is the maximum value in eV allowed for the FWHM of a peak.

RSAP searches for peaks in the total cross section data in the energy range specified and estimates the width, height, and area of each peak found. The data and a sum of SLBW (single-level Breit-Wigner) shapes are then plotted. RSAP writes an output file, **rsap.peaks**, containing a list of energy, gamma width Γ_γ , neutron width Γ_n , fission widths, and flags in the format of the SAMMY PARAmeter file. Estimates of the peak height σ_o , total width Γ , statistical factor g , and wave number k , are used to estimate Γ_n and the fission width, Γ_f .

$$4\pi g\Gamma_n = \sigma_o k^2 \Gamma$$

$$\Gamma_f = \Gamma - \Gamma_\gamma - \Gamma_n$$

After a peak search, the "**sam**" specifier will tell RSAP to create a SAMMY input file, **rsap.samin**, do a SAMMY Bayes run with the input PAR file **rsap.peaks**, and plot the results. An example input file is reproduced below.

```
ev 2
odf /home/ros/axp/RSAP/v5/EXAMPLE/11/u233temp.odf
tit PKFIND FWHM 1.1, BIAS 3
ops 1 1 1 0 1 1
### fwhm, bias, a2targ, Itarg, Jtot, gamgam, fwhmax
pks 1.1, 3.0, 235., 0.,0.5, 0.5, 1.2
x
1 etb 500.,516.,0.0,70.

sam
q
```

To run this example and plot on your X terminal (see Figure 11), type:

```
rsap < /home/ros/axp/RSAP/v5/EXAMPLE/11/tranxps
```

On the first plot (Fig. 11A) the solid line is the sum of SLBW shapes, and the dashed line is the SLBW sum plus a linear background computed from the first and last data points. On the second plot (Fig. 11B) the solid line is the SAMMY Bayes fit, and the dashed line is the SAMMY theory (initial theoretical value).

Figure 11A. /home/ros/axp/RSAP/v5/EXAMPLE/11/tranxps

Figure 11B. /home/ros/axp/RSAP/v5/EXAMPLE/11/tranxps

6. Automatic Spin Group Variation (SGV)

The process of fitting neutron cross section data with SAMMY often requires the user to try several spin values in order to obtain the best fit for a given resonance or group of neighboring resonances. Each trial requires several steps: a) editing the PAR file to change the spin group number, b) running SAMMY, c) viewing the results, and d) comparison with results from other trials.

An automatic spin group variation (**SGV**) procedure has been implemented in RSAP to facilitate the determination of spin group values for resonances. A simple RSAP input file allows the user to specify SAMMY input and PAR files, one or more resonances, an energy range for the fit, and up to 8 spin groups for each resonance. For each specified spin group, RSAP automatically edits the PAR file, runs SAMMY, and writes out CHISQ/NDAT and final resonance parameters. The required specifiers and their arguments are :

```
par SAMMY_PAR_file_name
sgi SAMMY_input_file_name
sgd SAMMY_data_file_name
sgr resonance_number, jsg1, jsg2, ..., jsg8      (a4, 9i4)
sgv esglo,      esghi                          (a4, 2f8)
```

The **resonance_number** corresponds to the record number in the PAR file, and **jsg1** is the spin group number to be used for the i^{th} SAMMY fit. The action specifier **sgv** tells RSAP to loop over the indicated spin groups, fitting over the energy range (eV) from **esglo** to **esghi**. If a plot is wanted, the user should insert **sgp** after **sgv**. An example file with resonance 25 and spin groups 3, 5, and 6 is reproduced below.

```
/home/ros/axp/RSAP/v5/EXAMPLE/12/dosgv25
```

```
par /home/ros/axp/RSAP/v5/EXAMPLE/12/o16/FINAL326.par
###          SAMMY input file
sgi /home/ros/axp/RSAP/v5/EXAMPLE/12/o16/cjav3ndsh_M5.in
###          SAMMY data file
sgd /home/ros/NUCDATA/sammy/o16/DATA/cj20742avg3normdsh.dat
###          resonance number, spin group numbers
sgr 25, 3, 5, 6
###          esglo,      esghi
sgv 4500000., 4610000.
###          automatic plot:
sgp
```

All parameters flagged in the user's original PAR file are varied in the SAMMY fits. RSAP does not modify the original PAR and INP files.

ODF and final PAR files for each spin group fit are saved in the subdirectory **00_00**, which is created by RSAP. A repeat SGV run causes **00_00** to be deleted and re-created. For the above example, the saved files are:

```
./00_00/SG_25_03.PAR      ./00_00/SG_25_03.ODF
./00_00/SG_25_05.PAR      ./00_00/SG_25_05.ODF
./00_00/SG_25_06.PAR      ./00_00/SG_25_06.ODF
```

The file names are written on the "**sgp**" plot as shown in Figure 12.A.

Figure 12A. `/home/ros/axp/RSAP/v5/EXAMPLE/12/dosgv25`

Fit results are written to files **rsap.chi** and **rsap.sgvout**:

RSAP SGV : Here is file rsap.chi

Resonance 25						

Resonance	Group	CHISQ/NDAT	Eres(eV)	Ggamma	Gneutron	
25	3	8.9857	4524740.526	2.5000E+02	6.3516E+06	8.8506E+05
25	5	0.6202	4527389.229	2.5000E+02	4.9415E+06	1.1957E+06
25	6	4.1012	4528243.660	2.5000E+02	4.6382E+06	1.1648E+06

RSAP SGV : Here is file rsap.sgvout:

Eres(eV)	Ggamma	Gneutron	Gfiss1	Gfiss2		
4524740.526	2.5000E+02	6.3516E+06	8.8506E+05		1 0 1 1	3 200.00
4527389.229	2.5000E+02	4.9415E+06	1.1957E+06		1 0 1 1	5 200.00
4528243.660	2.5000E+02	4.6382E+06	1.1648E+06		1 0 1 1	6 200.00

An alternate way of indicating sequential spin groups is illustrated by the command

sgr 25, -3, -7

This command tells RSAP to do SAMMY fits for spin groups 3 through 7 for resonance 25. Figure 12.B. shows output produced with the RSAP input file

/home/ros/axp/RSAP/v5/EXAMPLE/12/dosgv25__3thru7

Figure 12B. /home/ros/axp/RSAP/v5/EXAMPLE/12/dosgv25.3thru7

Resonance	Group	CHISQ/NDAT	Eres(eV)	Ggamma	Gneutron		
25	3	5.4591	4524764.278	2.5000E+02	5.9355E+06	7.4464E+05	
25	4	11.9090	4525554.599	2.5000E+02	5.4117E+06	4.7090E+05	
25	5	0.5497	4527397.612	2.5000E+02	4.9908E+06	1.1212E+06	
25	6	2.9556	4528284.932	2.5000E+02	4.7568E+06	1.1009E+06	
25	7	2.0291	4528261.389	2.5000E+02	3.6589E+06	2.2829E+06	

Eres(eV)	Ggamma	Gneutron	Gfiss1	Gfiss2			
4524764.278	2.5000E+02	5.9355E+06	7.4464E+05		1	0	1
4525554.599	2.5000E+02	5.4117E+06	4.7090E+05		1	0	1
4527397.612	2.5000E+02	4.9908E+06	1.1212E+06		1	0	1
4528284.932	2.5000E+02	4.7568E+06	1.1009E+06		1	0	1
4528261.389	2.5000E+02	3.6589E+06	2.2829E+06		1	0	1

6.1 Resonances treated sequentially.

Several resonances may be treated sequentially in one RSAP input file. An example RSAP input file for 2 sequential resonances is:

```
/home/ros/axp/RSAP/v5/EXAMPLE/12/dosgv__25then27

par /home/ros/axp/RSAP/v5/EXAMPLE/12/o16/FINAL326.par
sgi /home/ros/axp/RSAP/v5/EXAMPLE/12/o16/cjav3ndsh_M5.in
sgd /home/ros/NUCDATA/sammy/o16/DATA/cj20742avg3normdsh.dat
###                               1st resonance #, spin group numbers
sgr 25, 4, 5, 6
###   esglo,   esghi
sgv 4500000., 4610000.
###                               automatic plot:
sgp
###                               save ps file for 1st resonance
sys mv sgvl.ps sg25.ps
###                               2nd resonance #, spin group numbers
sgr 27, 6, 7, 8, 9
sgv 4600000., 4660000.
sgp
###                               save ps file for 2nd resonance
sys mv sgvl.ps sg27.ps
q
```

Fit results for the 2nd and subsequent resonances are appended to **rsap.chi** and **rsap.sgvout**. The above example file produces a total of 7 SAMMY runs, 3 for resonance 25 and 4 for resonance 27. Note also that a different energy range is used for each resonance.

6.2 Two Resonances treated simultaneously.

Two resonances may be treated simultaneously in one RSAP input file. In this mode RSAP does nested loops over spin groups:

```
Do j2=1,j2max      ! spin group loop for resonance 2
  Do j1=1,j1max    ! spin group loop for resonance 1

    Edit PAR file and run SAMMY

  enddo
enddo
```

By specifying the maximum of 8 spin groups for each resonance, 64 SAMMY runs could be performed.

An example RSAP input file for "simultaneous" resonances is:

```
/home/ros/axp/RSAP/v5/EXAMPLE/12/dosgv25and26

###          Vary spin groups for both res. 25 and res. 26
par /home/ros/axp/RSAP/v5/EXAMPLE/12/o16/FINAL326.par
sgi /home/ros/axp/RSAP/v5/EXAMPLE/12/o16/cjav3ndsh_M5.in
sgd /home/ros/NUCDATA/sammy/o16/DATA/cj20742avg3normdsh.dat
### resonance number, spin group numbers
sgr 25, 4, 5, 6, 7, 10
sgr 26, 8, 9
### esglo,      esghi
sgv 4500000., 4610000.
sgp
```

For this example, ODF and final PAR files for each spin group fit are saved in the subdirectories **26_08** and **26_09**. The saved files are:

```
./26_08/SG_25_04.PAR      ./26_08/SG_25_04.ODF
./26_08/SG_25_05.PAR      ./26_08/SG_25_05.ODF
./26_08/SG_25_06.PAR      ./26_08/SG_25_06.ODF
./26_08/SG_25_07.PAR      ./26_08/SG_25_07.ODF
./26_08/SG_25_10.PAR      ./26_08/SG_25_10.ODF

./26_09/SG_25_04.PAR      ./26_09/SG_25_04.ODF
./26_09/SG_25_05.PAR      ./26_09/SG_25_05.ODF
./26_09/SG_25_06.PAR      ./26_09/SG_25_06.ODF
./26_09/SG_25_07.PAR      ./26_09/SG_25_07.ODF
./26_09/SG_25_10.PAR      ./26_09/SG_25_10.ODF
```

The file names are written on the "**sgp**" plot as shown in Figures 12.C and 12.D.

Fit results are written to files **rsap.chi** and **rsap.sgvout**:

RSAP SGV : Here is file rsap.chi

Resonance 25		Resonance 26							
Resonance	Group	Resonance	Group	CHISQ/NDAT	Eres (eV)	Ggamma	Gneutron		
26									
8	25	4		17.8380	4525472.200	2.5000E+02	4.8743E+06	5.7239E+04	
8	25	5		0.6202	4527389.229	2.5000E+02	4.9415E+06	1.1957E+06	
8	25	6		4.1012	4528243.660	2.5000E+02	4.6382E+06	1.1648E+06	
8	25	7		3.0712	4528323.287	2.5000E+02	3.5306E+06	2.2838E+06	
8	25	10		6.0854	4527360.848	2.5000E+02	2.7106E+06	3.1953E+06	
9	25	4		19.2822	4525403.442	2.5000E+02	4.7154E+06	5.6229E+05	
9	25	5		0.6204	4527412.089	2.5000E+02	4.9870E+06	1.2924E+06	
9	25	6		4.0904	4528266.812	2.5000E+02	4.6799E+06	1.2451E+06	
9	25	7		3.0909	4528318.713	2.5000E+02	3.5743E+06	2.3120E+06	
9	25	10		6.1926	4527358.600	2.5000E+02	2.7273E+06	3.1474E+06

Figure 12C. /home/ros/axp/RSAP/v5/EXAMPLE/12/dosgv25and26

Figure 12D. /home/ros/axp/RSAP/v5/EXAMPLE/12/dosgv25and26

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REFERENCES

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2. M. J. LeBrun, G. Furnish, and T. Richardson, The PLPLOT Plotting Library, 1994.
<http://emma.la.asu.edu/plplot>
3. M. A. Mariscotti, Nucl. Inst. Methods **50**, 309 (1967).

APPENDICES

A. Example Script for SAMMY + RSAP Run

```

set sammy=/home/nml/m5/exe/sammy
set rsap=/home/ros/axp/RSAP/v5/gorsap5
#
#####                               make rsap input file for device x
cat <<eod> inx
par JohnFowl235_990203.par
odf SAMMY.ODF
tit JohnFowl235_990203 3.784                Title (a32)
ops 1 100 1 1 1
x
1 deb 2200.,2500.,0.0,1.00                (a2, a4, 4f10)

q
eod
#####                               make SAMMY input file
cat <<eod> input
/home/ros/NUCDATA/sammy/o16/990203/JohnFowl235.in
/home/ros/NUCDATA/sammy/o16/990203/JohnFowl235_990203.par
/home/ros/NUCDATA/sammy/o16/DATA/JohnFowl235_HC981111.dat 2285000.0,2490000.

eod
$sammy < input > output
#
$rsap < inx

```

B. Example **rsap.ratexpth** File

E(keV)	SigmaExp(b)	Error(b)	Theory(b)	BAYES(b)	100* (Th/Exp-1)	100* (BAYES/Exp-1)
200.8193	3.4680E+00	0.02500	3.50496E+00	3.50464E+00	1.066	1.056
201.8257	3.4620E+00	0.02570	3.50363E+00	3.50331E+00	1.203	1.193
202.8397	3.4020E+00	0.02570	3.50231E+00	3.50198E+00	2.949	2.939
203.8613	3.4740E+00	0.02550	3.50099E+00	3.50066E+00	0.777	0.768
204.8908	3.4410E+00	0.02500	3.49968E+00	3.49935E+00	1.705	1.696
205.9279	3.4510E+00	0.02440	3.49837E+00	3.49804E+00	1.373	1.363
.....						
6200.874	9.6110E-01	0.13790	9.40398E-01	9.41881E-01	-2.154	-2.000
6211.689	1.0610E+00	0.13970	9.32850E-01	9.34306E-01	-12.078	-11.941
6222.533	9.5580E-01	0.13670	9.25973E-01	9.27403E-01	-3.121	-2.971
6233.404	9.9550E-01	0.13940	9.19679E-01	9.21084E-01	-7.616	-7.475

C. Example **rsap.parcom** File

Wed Jan 27 14:46:35 EST 1999

duanesh_990126.par

Res	Grp	E(keV)	E/SAM	GamC1	GamC1/SAM	GamC2	GamC2/SAM	Vary	Eunc.
1	1	-12024.00	-12021.00	9106.20	9126.20			1 0 1	10.0
2	1	-4469.30	-4469.20	5469.30	5485.00			1 0 1	1.0
3	3	434.30	434.30	44.17	44.40			1 0 1	0.2
4	4	1000.28	1000.25	99.64	100.43			1 0 1	0.2
5	3	1309.36	1309.36	43.17	43.35			1 0 1	0.2
.....									
37	6	6076.13	6076.13	4.76	4.81	2.00	2.00	1 0 1	0.2
38	2	6087.91	6087.90	14.53	14.57	4.51	4.51	1 0 1	0.2
39	7	6387.66		9.91	10.01	35.98	36.01	0 0 0	0.2
40	3	10980.19	10989.91	14338.00	14369.00			1 0 1	100.0
41	2	18777.06	18755.84	27453.00	27495.00			1 0 1	100.0
42	4	16158.63	16146.03	1926.00	1930.90			1 0 1	100.0

RADIUS PARAMETERS FOLLOW

3.77736 3.7773611-1 1 2 3 4 5 6 7 8 0 1
6.49920 6.4992011-1 1 2 3 4 5 6 7 8 0 2

NORMALization and "constant" background follow

1.0038828 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1 0 0 0 0 0

COVARIANCE MATRIX IS IN BINARY FORM

Grp	Res	er	gam	samer	samgam	samgam2	
1	1	-12024.000	9106.200	-12021.000	9126.200	0.000	s1/2
1	2	-4469.300	5469.300	-4469.200	5485.000	0.000	
1	3	2378.121	160.770	2377.930	160.360	0.000	
.....							
7	1	1651.380	4.004	1651.380	4.053	0.000	f7/2
7	2	3766.949	18.148	3766.947	18.350	0.015	
7	3	5123.835	22.531	5123.806	22.761	2.016	
7	4	6387.658	9.912	6387.658	10.006	36.010	
8	1	4594.304	1.492	4594.304	1.515	0.203	g7/2
8	2	5918.549	19.342	5918.571	19.624	2.501	
Grp	Res	er	gam	samer	samgam	samgam2	
CUSTOMARY	CHI SQUARED DIVIDED BY NDAT	=	1.53943				
CUSTOMARY	CHI SQUARED DIVIDED BY NDAT	=	1.48805				
CUSTOMARY	CHI SQUARED DIVIDED BY NDAT	=	1.48802				

D. PLPLOT metafiles and `plrender`

The discussion herein follows closely the information given in the PLPLOT documentation [2]. A PLPLOT metafile is a binary, device-independent stream of bytes that may be rendered with the PLPLOT utility, `plrender`.

To render the metafile, `rsap.meta`, type:

```
plrender [options] rsap.meta
```

where

options(partial list):

<code>-dev name</code>	Output device name
<code>-o name</code>	Output filename
<code>-px number</code>	Plots per page in x
<code>-py number</code>	Plots per page in y
<code>-geometry geom</code>	Window size, in pixels (e.g. <code>-geometry 400x300</code>)
<code>-wplt xl,yl,xr,yr</code>	Relative coordinates [0-1] of window into plot
<code>-mar margin</code>	Margin space - relative coord (0 to 0.5, def 0)
<code>-a aspect</code>	Page aspect ratio (def: same as output device)
<code>-jx justx</code>	Page justification in x (-0.5 to 0.5, def 0)
<code>-jy justy</code>	Page justification in y (-0.5 to 0.5, def 0)
<code>-ori orient</code>	Plot orientation (0,2=landscape, 1,3=portrait)
<code>-bg color</code>	Background color (0=black, FFFFFFFF=white)

All parameters must be white-space delimited. Not all options valid with all drivers.

A complete list of options may be obtained by typing “`plrender -h`”.

For example, to make a color postscript file, `rsap_port`, in portrait orientation on a white background:

```
plrender -dev psc -bg FFFFFFFF -o rsap_port -ori 3 rsap.meta
```

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