
sizes Documentation

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Pete R. Jemian

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author Pete R. Jemian

email jemian@anl.gov

URL <http://prjemian.github.io/sizes>

git <https://github.com/prjemian/sizes>

<p>Caution: Python version is not complete.</p>
--

The Python version of the *sizes* program (for size distribution analysis of small-angle scattering data using the maximum entropy method of Skilling and Bryan) **is under construction**. Not all features of the C and FORTRAN versions of the code are yet available.

The documentation for this version is rudimentary, as well.

The manual for the FORTRAN version is available: [guide.pdf](#) as well as a previous version of the FORTRAN documentation in the section here titled: *USER GUIDE FOR THE MAXIMUM ENTROPY SAS ANALYSIS PROGRAM MaxSas.for*.

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1.1 About sizes

1.1.1 License

This software is licensed using the Argonne OPEN SOURCE LICENSE, see LICENSE file for details

1.1.2 Change History

This describes user-visible changes between the versions.

This program is a translation from the C which is from the FORTRAN which is from the BASIC version.

Version 2013-05

initial translation from C code

Credits:

- P.R. Jemian, Argonne National Laboratory, USA

Used in Irena package

An IgorPro translation of this code appears in the *Irena* software package, authored by Jan Ilavsky. [cite publication history here]

Credits:

- Jan Ilavsky, Argonne National Laboratory, USA
- P.R. Jemian, Argonne National Laboratory, USA

C translation

The FORTRAN code was translated into C ca. 1990.

Credits:

- P.R. Jemian, Northwestern University, USA

Previously

This program was written in BASIC by GJ Daniell and later translated into FORTRAN and adapted for SANS analysis. It has been further modified by AJ Allen to allow use with a choice of particle form factors for different shapes. It was then modified by PR Jemian to allow portability between the Digital Equipment Corporation VAX and Apple Macintosh computers.

Credits:

- G.J. Daniell, Dept. of Physics, Southampton University, UK
- J.A. Potton, UKAEA Harwell Laboratory, UK
- I.D. Culverwell, UKAEA Harwell Laboratory, UK
- G.P. Clarke, UKAEA Harwell Laboratory, UK
- A.J. Allen, UKAEA Harwell Laboratory, UK

1.2 maximum entropy calculation engine

The 1984 Skilling and Bryan paper is available online ¹ through the SAO/NASA ADS Astronomy Abstract Service:

1.3 main source code module: *sizes*

1.4 USER GUIDE FOR THE MAXIMUM ENTROPY SAS ANALYSIS PROGRAM MaxSas.for

author Pete R. Jemian, Northwestern University, 7 February 1990

Substantial portions of this document are from the documentation supplied with the code MAXE (documentation by Ian Culverwell, UKAEA-Harwell, 23 February 1987) and with its modification called MAXE2 (modifications by Andrew Allen, UKAEA-Harwell, 19 July 1989).

Contents:

1.4.1 INTRODUCTION

This program provides an accurate and reliable analysis of small-angle scattering data. Using an iterative approach it calculates the size distribution of scatterers of a specified form, with the maximum entropy, whose scattering pattern is consistent with the data. The consistency test is the ChiSquared statistic. A full description of the program's methodology and of its rigorous validation can be found in [Culverwell, 1986] and [Potton, 1988a].

¹ <http://adsabs.harvard.edu/abs/1984MNRAS.211..111S>

The MaxSas code is an interactive program, and users must be prepared to answer the questions that the program will ask. The questions are grouped into two major sections: input data selection and scattering model selection. The input data selection is by file name and Q-vector range. The scattering model selection is by form factor, diameter range, and number of histogram bins. It may be necessary to run this program several times, with slight changes in user-adjustable parameters, in order to obtain a satisfactory analysis.

The running of the program will be demonstrated by example, using synthetic scattering data calculated from a hypothetical bimodal particle size distribution (ref 3). This distribution consists of a narrow Gaussian peak centered at 80 Angstroms with a standard deviation of 20 A, together with a broader secondary Gaussian peak, half the size of the primary one, centered at 200 A with a width of 60 A. In order that they can become familiar with the questions that the program will ask them, prospective users are advised to run the program using this data set, reproducing verbatim the example responses quoted in this guide.

1.4.2 INPUT DATA FORMAT

The input data file should be in the same format as in the supplied synthetic scattering data (file: BIMODAL.SAS). Formally the data should exist in the file as ordered triples of scattering vector (in 1/A), intensity and estimated error of intensity. Typically, the data will be in three columns, separated by “white space” of spaces and/or tabs. The intensity may be in any units as the program will ask for a conversion factor between these units and 1/cm units. The numbers are read as floating point numbers, hence 0.0015, 1.5E-3, 0.15E-2, and 15E-4 will be identical. However, do not be tempted to force double precision input (such as 1.5D-3) because this may provoke a nasty error condition.

The name of the data set should any standard filename for the operating system on which the program is run. A typical name would be BIMODAL.SAS (the synthetic scattering described earlier) which describes bimodal SAS data. If the data file resides in a directory other than the default, then you will have to specify that as part of the file name. Example file names, including a “full path description” follow for the more popular operating systems:

Digital Equipment Corporation VAX running VMS:

```
DISK$MPD_USERS: [CULVERWEL.MAXE] BIMODAL.SAS
```

Apple Macintosh:

```
Hard Drive:MaxSas Folder:test case:BIMODAL.SAS
```

MS-DOS computer (such as the IBM-PC):

```
C:\MAXSAS\TEST\BIMODAL.SAS
```

1.4.3 OUTPUT FORMAT

One output file is created by the program - a data file whose name is user supplied (e.g. BIMODAL.MAX).

The first few lines of output of a typical output file are as follows:

```
Results of maximum entropy analysis of SAS
  version 3.1 (PRJ)                , edited:7 February 1990

input file:   Bimodal.Sas
output file:  Bimodal.Out
-----

N(D) dD is number of particles/cm**3
      whose size is between D and D + dD

      D, A          V(D)*N(D), 1/A          N(D), 1/A/cm^3          dD, A
      ----          -
      -----          -----          -----          -----
```

10.00	8.81630E-15	1.68379E+07	10.0000
20.00	2.16369E-14	5.16543E+06	10.0000
30.00	6.36171E-14	4.49999E+06	10.0000

The four columns are separated by TABs and also spaces.

term	description
D	dimension of scatterer in Angstroms
V(D)*N(D)	volume-weighted differential number distribution
N(D)	differential number distribution
dD	width of the bin in Angstroms in terms of "D"

V(D)*N(D) is the distribution solved by the program. N(D) is the distribution most often reported by other analysis techniques (TEM, mercury porosimetry, etc.). N(D) is calculated from the second one by dividing by the particle volume. This table continues as:

380.00	8.11590E-07	2.82480E+10	10.0000	
390.00	5.74524E-07	1.84976E+10	10.0000	
400.00	3.71052E-07	1.10728E+10	10.0000	
Q 1/A	I 1/cm	^I 1/cm	dI 1/cm	z
-----	-----	-----	-----	-----
7.4936E-03	2.1200E+00	2.2330E+00	1.6700E-01	-0.676923
9.9975E-03	1.9000E+00	1.9596E+00	1.0200E-01	-0.584780
1.2501E-02	1.7840E+00	1.6605E+00	6.6900E-02	1.845438

These columns are also separated by a combination of spaces and tabs

term	description
Q	input Q-vector in 1/Angstrom units
I	input intensity in 1/cm units
^I	intensity calculated from the distribution above
dI	input error in 1/cm, scaled by the error scaling factor
z	standardized residual, $z = (I - ^I)/dI$

9.2452E-02	4.3770E-03	4.2886E-03	1.6700E-04	0.529397
9.5008E-02	3.4510E-03	3.7178E-03	1.5000E-04	-1.778752
9.7564E-02	3.5330E-03	3.2077E-03	1.3500E-04	2.409922
9.9937E-02	2.9560E-03	2.7793E-03	1.2300E-04	1.436465
Input data: Bimodal.Sas				
Contrast = 1.0000000 x 10^28 m^-4.				
spheroid: D x D x D* 1.00000000000000				
Data conversion factor to 1/cm = 1.00000E+00				

After all the intensities have been printed, the same summary appears in the output file as appeared on the screen shown above. Only the first few lines are shown here.

The program creates two extra pseudo-particle sizes, one that is "smaller" than the smallest bin in the distribution and one that is "larger" than the largest bin in the distribution. The scattering from these pseudo-particles is approximated at low angles by the Guinier relation and at high angles by the Porod relation. The object of the user is to define the dimension range large enough that neither of these pseudo-particles develops any significant volume fraction. The percentage of the distribution that was assigned to each of these sizes is reported. Provided that both are small compared to the total volume fraction of scatterers (also given in the summary) then the program has detected essentially all of

the particles contributing to the observed scattering. If they are not, it may be worth re-running the program with a different diameter range in order to detect this extraneous volume fraction.

1.4.4 EXAMPLE OF THE PROGRAM EXECUTION ON A DEC Vax

The following is an excerpt from the execution of MaxSas as it is analyzing the supplied test distribution BIMODAL.SAS, a bimodal distribution with two Gaussian peaks: one at 80 Angstroms with a sigma of 20 A and the other at 200 A with a sigma of 60 A. The Gaussian at 200 A is half the height of the one at 80 A. For a further discussion of this distribution, see [Culverwell, 1986]. The exact volume fraction of the original distribution was not specified.

In the section to follow, all user responses will be all in upper case where appropriate and will be followed by a {CR}, signifying that the user has pressed the return key. {CR} by itself signifies that the user has accepted the default answer to the question, as shown in <default>. Almost all questions have a default response, the only exception being the output file names which may take any value EXCEPT blank or the same as the input file name. Initially, all the defaults are preset to the proper answers for the supplied test distribution BIMODAL.SAS. If you type in a new value, that will value will become the default the next time that the question is asked.

The example to follow will be interrupted from time to time for explanations. These will be isolated between rows of "====" signs. For further explanations of each question which is asked, see the appropriate section appearing elsewhere in this document.

Now here's the excerpt from the beginning of the run. Remember that all user responses are on a single line and are terminated with a {CR}.

```

$ RUN MaxSas{CR}

Size distributions from SAS data using the maximum entropy criterion
  version: 3.1 (PRJ)           ,    7 February 1990
Input file? <Quit>
Bimodal.Sas{CR}
Output file?
Bimodal.Out{CR}
Minimum q-vector? [1/A] < 1.0000000000000000E-008>
{CR}
Maximum q-vector? [1/A] < 100.0000000000000    >
{CR}
Scattering contrast? [10^28 m^-4] < 1.000000000000000    >
{CR}
Factor to convert data to 1/cm? < 1.000000000000000    >
{CR}
Error scaling factor? < 1.000000000000000    >
{CR}
Background? < 0.0000000000000000E+000>
{CR}
Spheroids: D x D x vD, Aspect ratio (v)? < 1.000000000000000    >
{CR}
Bin step scale? (1=Linear, 2=Log) < 1>
{CR}
Number of histogram bins? < 40>
{CR}
Maximum value of D? [A] < 400.0000000000000    >
{CR}
Minimum value of D? [A] < 10.000000000000000    >
{CR}
Maximum number of iterations? < 20>
{CR}

```

```

Reading from file: Bimodal.Sas
      38 points were read from the file
      38 points were selected from the data
Preparation of the GRID function...
Setting BASE constant at 1.0000000000000000E-012
MaxEnt routine beginning ...
    
```

To recap what has happened so far, the program was started and the input data file BIMODAL.SAS was specified for analysis. All the default answers appeared to be acceptable so the program read 38 points from the file, of which all 38 points were retained for the analysis. The program informs you that it has set an internal array called BASE to 1.0E-12. BASE is the initial guess for the distribution. If there is a value in the output distribution that is comparable with this number, then that particular histogram bin has no significant information. Consider then that BASE is the “featureless” distribution and rest assured that it is quite flat.

At this point, the program has gotten all the adjustable parameters that it needs and is now proceeding to attempt to solve the problem.

The fitting routine is an iterative one. If there are N histogram bins and P data points then the computation time for each iteration will be on the order of (very approximate) $\text{Order}(2N+P)$. (This is why both N and P are bounded.)

All sorts of information will begin to scroll on the screen at an alarming rate as the Maximum Entropy routine, or MaxEnt, (see [Skilling, 1984] for details on what’s happening) begins to extract statistically significant information from the SAS data. With each iteration, several different types of screen plots are drawn, each describing the data extracted so far. The different plots are titled:

- LOG (ChiSq) vs. iteration number
- Entropy vs. iteration number
- Residuals
- Distribution

The first two plots will not appear until the third iteration. They are intended to keep you informed about the progress of the MaxEnt routine. The residuals (difference between MaxEnt fit and input data normalized to the input errors) are plotted as a function of data point subscript number, not Q-vector. The distribution is weighted by the bin width, $dD(i) = D(i+1) - D(i)$, and is also plotted as a function of diametral bin subscript number. All plots will be scaled to fit within the screen boundaries.

The last information to appear in each iteration will be a report, such as:

```

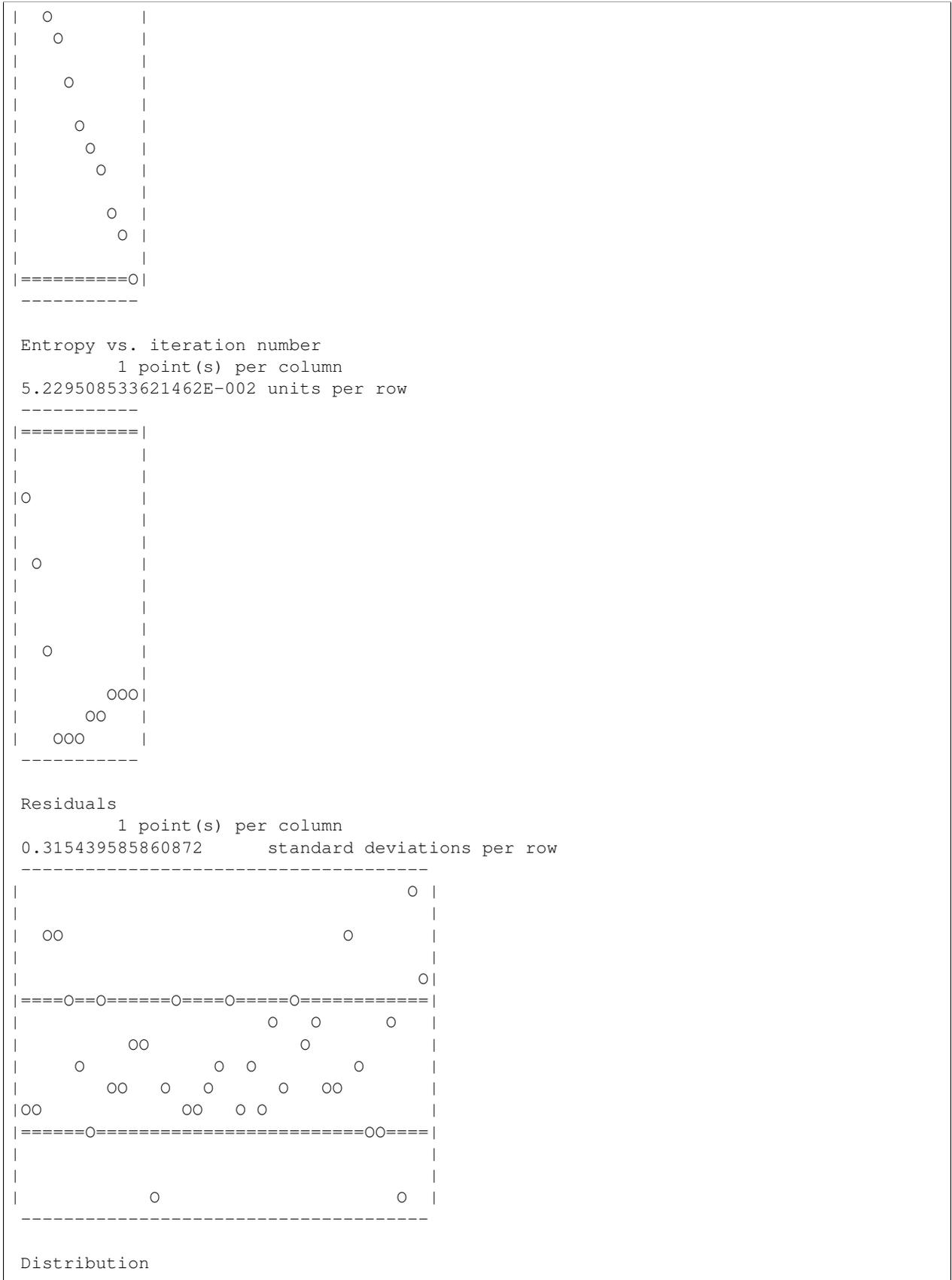
#          2 of          20,  n =          38
test =    0.19101,  Entropy =    3.4668138
SQR((Chi^2)/n):  target = 12.14204774    % off =    26.2698
f-vector:      sum =    0.00452313    % change =    0.4663
    
```

The report is saying that for the second iteration out of 20, where there are 38 intensity data points, the difference between the entropy and ChiSquared gradients is 0.19101, the entropy of the distribution just plotted is 3.4668138 (whose units are exact), the target for the $\text{SQR}((\text{ChiSquared})/n)$, where ChiSquared is derived from intensity calculated from the distribution just plotted, of 12.14204774 was missed by 26.2698%, and the total volume fraction of scatterers in the distribution just plotted is 0.452313 %, which did not change much from the previous iteration. The iterations will continue.

Here is the screen output from the last iteration:

```

LOG (ChiSq) vs. iteration number
      1 point(s) per column
0.405168291335942    units per row
-----
|                   |
|00                 |
    
```




```
The change in ChiSquared should be < 5%.
Run the Stability Check? (Y/<N>)
Y{CR}
Setting BASE constant at      1.0000000000000000E-12
MaxEnt routine beginning ...
```

For this documentation, the results of the stability check will not be shown. There is not much change in the volume fraction after the stability check (about 1% or so) for the supplied test distribution.

After the Stability Check, you should get this question again. This time, respond like the following to quit the program.

```
The change in ChiSquared should be < 5%.
Run the Stability Check? (Y/<N>)
{CR}

The program is finished.
The output file is: BIMODAL.MAX

Size distributions from SAS data using the maximum entropy criterion
  version: 3.1 (PRJ)           ,    7 February 1990
  Input file? <Quit>
{CR}
$
```

1.4.5 User Interaction with the program

A FEW WORDS ABOUT NUMERICAL RESPONSES BY THE USER

If you respond to a numerical question with a “zero”, the default answer will be used. That is the way this program works to give you default answers. If you want to set a parameter to be “zero”, use an infinitesimal value such as 1.0E-25.

All floating point responses should include a decimal point somewhere in the mantissa of the response, otherwise the results are unpredictable and very system dependent!

EXPLANATION OF QUESTIONS ASKED BY THE PROGRAM

Q: Input file? <Quit>

The input file contains the SAS intensity data as ordered triples of Q-vector (in 1/A units), Intensity (in arbitrary units), and statistical error of intensity (same as intensity units). Note that there are no initial header lines in the input file. No more than the first 300 data points (ordered triples) will be read from the input file.

If you were to press {CR} without typing in a file name, the program would quit (as indicated by the default).

If the input file does not exist, the program will happily proceed to ask you all the remaining questions it has. Then and only then will it find out that the file you named does not exist. This will generate a program crash.

A suggestion for input file name extensions is “.SAS” but this only a suggestion. The input file name may be up to 80 characters long.

Q: Output file?

This is the only question which has no default answer. You must answer this question with something. If your answer is the same as the input file name, the program will start over asking you for the input file name. This may be used as an easy exit if you specified the wrong name.

The program does not check to see if the named output file already exists. On some systems (Macintosh and MS-DOS), the old file will be erased and a new file created. On other systems (VAX), a file with the same name but a new version number will be created. Forewarned is forearmed.

My suggestion for MaxSas solution file name extensions is ".MAX" or ".DIS". The output file name may be up to 80 characters long.

Q: Minimum (Maximum) q-vector? [1/A]

Use Q-vector (actually Q-vector magnitude) in units of 1/Angstrom. The user is allowed to exclude data points from the ends of the input data. Only those data points satisfying $q_{\text{Min}} \leq Q\text{-vector} \leq q_{\text{Max}}$ will be analyzed. The program is designed to only handle positive Q-vectors.

Initially, q_{Min} is set ridiculously low so that even the lowest data point will be used. Correspondingly, q_{Max} is set high enough to include all typical SAS Q-vectors.

The user should generally cut off the data when the signal-to-noise ratio becomes poor. Truncating earlier than this will lose information about the smallest particles present in the sample. Users might note that it is not necessary for all the intensity values to be positive, although it is probably inadvisable to include more than five negative ones.

Q: Scattering contrast? [10^{28} m^{-4}]

The scattering contrast is the squared difference between the scattering length density of particle and matrix. If the contrast is $1.27\text{E}30 \text{ 1/m}^{**4}$, then enter the value 127.0. By the way, $1.27\text{E}28 \text{ 1/m}^{**4} = 1.27\text{E}20 \text{ 1/cm}^{**4}$.

The user can either enter the true contrast here or reply {CR}, in which case the final "volume fractions" obtained will have to be divided by the contrast (in units of $1.27\text{E}28 \text{ 1/m}^{**4}$) in order to obtain genuine volume fractions. The program is coded to accept scattering contrast values no larger than one million units of $1.0\text{E}28 (1.0\text{e}34) \text{ 1/m}^{**4}$.

Q: Factor to convert data to 1/cm?

If the intensity values in the input file were not in units of 1/cm, enter the constant to convert them into such units. If they were already in 1/cm units, good for you, so just press {CR} to accept the default. The program is coded to accept conversion values no larger than 1000.0.

Q: Error scaling factor?

Here is an opportunity for you to try analyzing your data with different ratios of signal to noise. If you think that the errors in the input file were underspecified, you may multiply them by this constant. More on this later as this will have a major influence upon the analysis.

Q: Background?

This program has left you the opportunity to subtract a constant intensity value. A good initial approximation will put you on the road to a good analysis of the data. Remarkably, the background may take any value, positive or negative. If you want to set the background back to zero, use infinitesimal (such as $1.0\text{E}-25$) rather instead. More on background later.

Q: Spheroids: D x D x vD, Aspect ratio (v)?

The scattering form factor currently implemented is that discussed by [Roess, 1947]. A special case of this ellipsoid of revolution, whose outside dimensions are D x D x vD, is the sphere whose form factor is described in [Culverwell, 1986] and [Potton, 1988a].

It is possible to select any aspect ratio (within reason) using this model and the program only checks to see that you have entered a positive value. Special care has been taken to ensure that the volume fractions determined by this model are correct.

For a full explanation of the coding of this model (from eq. 4, 5, & 6 of [Roess, 1947]), see the source code listing. Look for the routine named "Spheroid."

Remember that the distributions that are output are in terms of the dimension "D". The volume of this type of spheroid is $(4\text{Pi}/3) v \text{ r}^{**3}$.

Q: Bin step scale? (1=Linear, 2=Log)

“Linear” binning means that the diametral bins will increase in size according to an algebraic series (e.g. 1, 2, 3, ...). The other method currently available is “logarithmic” binning where the increase is according to a geometric series (e.g. 1.0, 1.05, 1.1025, ...). Use whichever method gives you a sufficient number of points over all the peaks in the distribution. Be aware that the calculated volume fractions and number densities for the first few bins on the “log scale” are likely to be artificially high because of the small bin width and small particle volume corresponding to that bin (both these terms divide the quantity that MaxSas derives to give you the volume fraction”).

The width of each bin indexed by “i” is $dD(i) = D(i+1) - D(i)$ so that the number density of scatterers whose size is between D and $D + dD$ is truly $N(D) dD$. The bin width appears in the output file as “dD.”

Q: Number of histogram bins?

This is an integer between 2 and 100, limited by computer memory and execution CPU time. Use as few bins as you think you need to adequately describe the distribution or as many bins as you want, up to the maximum of 100.

Q: Maximum (Minimum) value of D? [A]

Use Angstrom units. Because each intensity is a statistical representation of ALL dimensions D in the sample, weighted by a particular form factor (model function), the choice of maximum and minimum D is left to the user. You may specify values that are beyond the “peripheral vision” of your data to see if there is any statistical support for such sizes in your data. Usually, one knows something about the size distribution to be solved and a maximum particle diameter can be estimated. Ideally D_{max} should be an over-estimate; if too small a diameter range (D_{min} to D_{max}) is specified, the program will likely fail.

The largest value for D_{max} is something unreasonable for most SAS data (1 million Angstroms). If you try to exceed this limit, the program will patiently ask you again for the maximum D value. The smallest D_{min} value you may enter is 1.0 Angstrom. The program will always suggest $D_{min} = D_{max} / (\text{number of bins})$.

If $D_{min} \geq D_{max}$, the program will start asking you questions all over. You can use this as an easy way to correct a bad input prior to this question, without having to stop and restart the program.

Q: Maximum number of iterations?

The number of iterations is best estimated by experience. Skilling and Bryan [Skilling, 1984] suggest that one should re-consider the model if more than about 20 iterations are required for convergence within the Maximum Entropy routine (MaxEnt). The largest allowed number of iterations is 200 but if you require this, your model is probably not representing the data well. The MaxEnt routine may not require as many iterations as you specify. That just means the job was easier than you “thought”.

If, while the MaxEnt routine is iterating, you see that a few more iterations will be required to achieve a satisfying solution than you have specified here, all is not lost. If the limit specified is reached with no satisfying maximum entropy solution yet in hand, the program will ask you if you want to iterate more. You can then extend the process. For this reason, it is suggested that you specify a lower value (rather than higher) so that you may check the program’s progress. A low limit allows the MaxEnt routine to escape should the fitting process fail to converge. In such an event, one or more of the input parameters should be adjusted to achieve a more harmonious solution.

A good general suggestion for the number of iterations is the maximum number that you are willing to see the MaxEnt routine perform and not converge. If the MaxEnt routine needs more iterations, it will ask you for permission.

Q: The change in ChiSquared should be < 5%.

Run the Stability Check? (Y/<N>)

The Stability Check will perform the same analysis on the data set with all the same parameters except that the suggested background will be used. If the answer is stable, then all the results should be the same. If the answer is unsteady, then things will look different in some way. The prompt for a stability check will not appear unless the program calculates that the shift should produce less than a 5% change in the ChiSquared.

Q: Maximum iterations have been reached.:

```
How many more iterations? <none>
```

This question occurs inside the MaxEnt routine when the maximum number of iterations that you specified have been reached. If you want the MaxEnt routine to keep trying, specify a positive integer, otherwise take the default which will generate the following output:

```
No convergence! # iter. = "IterMax"
File was: "InFile"
```

The program will then start over at the first question.

1.4.6 SCREEN PLOTS

LOG (ChiSq) vs. iteration number

This plot will appear after the second iteration of the MaxEnt routine. If the ChiSquared is nearly constant for 3 or more consecutive iterations, this plot will not appear. The “====” bar in the plot indicates the target value of “N”, the number of intensity points.

Entropy vs. iteration number

This plot will appear for every iteration after the second. The “====” bar in the plot indicates the entropy of a flat distribution with the same number of diametral bins as have been specified.

Residuals

The standardized residuals are the difference between the intensity that is calculated from the distribution and the input intensity, all divided by the input error. For the model to fit the data well, this plot should look featureless (a.k.a. random). The “====” bars are at +1 and -1 standard deviations. 67% of the points should fit within the bars. If there is some systematic difference between the model and the data, the residuals will reveal it by showing some shape.

Distribution

The distribution plot appears at the end of each iteration and shows the most recent distribution, whose calculated intensity is to be compared with the input intensity and errors. The values in this plot are weighted (multiplied) by the bin width. This means that when the bins are distributed in a geometric series, it will be quite difficult for the user to see a small peak at smaller diameters in this plot. Have no fear though because this method weights the volume fraction in a manner equal to that of the algebraic series.

Volume weighted size dist.: $V(r)N(r)$ versus r

Once the MaxEnt routine has decided that it has a solution, this plot will appear. The vertical scale is the volume distribution (technically the “volume-weighted differential number distribution”). This is almost the same value as was plotted in the “Distribution” plot except the bin width has been divided out. The horizontal scale is a linear axis on which is plotted particle radii.

Note: The MaxEnt routine does its work with respect to particle radii. All answers are properly scaled to diametral units in the output files. Additionally, the MaxEnt routine works with intensities in 1/m units. It seems to do some bad things when the intensities are in 1/cm. The FORTRAN code isolates the user from this eccentricity. All unit conversions are corrected in the output data.

1.4.7 OBSERVATIONS, HINTS, SUGGESTIONS

Stability Check of the Solution

In the example case above, a second analysis of the test distribution was made to check the stability of the solution. This is a very good suggestion and is a must before you should present any data which you have analyzed. The stability check is made after a successful solution has been obtained by re-analyzing with no parameters changed except for the experimental background which the program suggests. If the answer is to be believed, the Stability Check should complete with a comparable number of iterations and determine a comparable background, volume fraction, and size distribution.

Getting the Background Close

It seems that there is a narrow thread on which the program may obtain a reasonable analysis (within 20 iterations). That thread has two adjustable parameters: error scaling and constant background. With a larger error scaling term, the exact value of the background is less important. If one is not certain of the background level (and some of the particle form models require a background different even from the experimental background), it can be very difficult to guess within the 10% or so required with an error scaling factor of unity.

An algorithm that seems to navigate that thread to an acceptable solution of a size distribution from a set of intensity data is as follows: Decide upon the aspect ratio and the largest range of dimensions that may exist in the data. Run the analysis, choosing all the data that you think will fit the model well. Specify the contrast if you know it. Increase the errors by a factor of 5.0 (or maybe 10, if conditions suggest). Take a guess at the background (the zero-order guess is zero). Let the MaxEnt routine try to solve the puzzle. If it does not converge within 20 iterations, increase the error scaling factor by double. Keep doing this until the MaxEnt routine says it has a “solution”. Good! We are not interested in this solution because the residuals probably look like a smooth, curved function. What we are trying to do is get the program to tell us what it “thinks” the background should be. Now that the program has suggested a background to us, try analyzing again with this background and a slightly decreased error scaling factor. Now we are on the “thread”. Keep bringing the error scaling factor down (I know this takes time) until you can be satisfied that the errors are well-specified or that there is some systematic reason why the model does not fit the data well. Whatever the background ends up as when you are satisfied with the error scaling factor, accept it and reanalyze the data again, leaving out any intensities that would be below that background.

The background suggested by the program is based on a statistically-weighted average of the difference between the intensity calculated from the distribution (\hat{I}) and the input intensity data (I). The exact equation looks like, where “s” are the input errors:

$$\text{NewBkg} = \text{Bkg} + \text{AVERAGE} ((I - \hat{I}) / s^{**2})$$

FAILURES

In ideal circumstances when the program is iterating successfully the user will observe the value of ChiSquared diminishing until it closely approaches its final target value, which is the total number of data points being used. Then in the final few iterations the entropy, which had been steadily decreasing, will be seen to increase. The residuals will become more randomly distributed with each iteration (a sign of a good fit to the data) and the size distribution will slowly converge to its final form. The program will then exit from the fitting routine. This is the behaviour observed when the program is run using the example data set.

It is quite possible for the fitting routine to fail to converge at the first attempt. If this happens the program will return to the calling routine after it has completed the maximum number of iterations specified in the input section above and display the following message:

```
No convergence! # iter. = "MaxIter"  
File was: "InFile"
```

The program will then return to the input section to begin a new analysis.

There are a number of problems which can arise. Some of these are annoying bugs in the program which are gradually being sorted out. The usual symptoms of trouble are:

1. **the program suddenly suffers ‘divide’ or ‘square-root’** execution errors
2. **it gets caught in a perpetual loop** (Hopefully, these errors have been trapped or corrected. The bulk of them are from passing a literal variable as a parameter to a subroutine or function. The size of the argument

is implied by the caller but actually specified, sometimes differently, by the called subroutine or function. The error is then, “passing the wrong size argument on the stack” which has been corrected by setting a variable, of known size, to the value of the literal and then passing the variable.)

The following remedies should be considered:

1. **take out points at either end of the data to change the program’s** calculation trajectory
2. change the size range or number of bins to have the same effect
3. **consider that ChiSquared is being pushed too hard so the error** scaling can be increased and the point of tragedy is never reached
4. adjust the constant background
5. **re-assess the DISTRIBUTION of assigned errors on the input** data – Do they reflect the true scatter ?
6. re-assess the particle form model with regard to the system
7. **is the scattering just too weak or noisy for a respectable program** like this one ?

Considerations (1)-(3) should resolve matters if you have encountered one of the program bugs; if not, then (4)-(7) may apply. In most situations, time spent adjusting the flat background seems to give the best return on effort expended. However it is worth considering a few points relevant to (6) above. The basic assumption is that the scattering system comprises a DILUTE assembly of identically shaped scattering particles, all of one kind, suspended in a uniform medium or matrix. Inter-particle interferences due to close packing at high concentrations are not presently considered. (J.E. Epperson is trying to develop methods for treating these.) Such inter-particle interferences are likely to result in run-failures or fictitious size distributions. A disordered interconnecting scattering interface within the sample may also lead to spurious results. Also the aspect ratio, cannot be determined from SAS data alone: if a size distribution can be obtained with one value, then size distributions should be equally obtainable over all realistic values for a given scattering particle type. Thus both the choice of shape function and the aspect ratio should be determined from independent methods such as electron microscopy, theoretical models etc.

ERROR SCALING

The most likely reason is that the quoted errors are too small to allow a close fit to the data by an algorithm that uses the ChiSquared test as its consistency criterion. This would probably be the case if, during the iterations, the user observed chi-squared asymptotically approaching a final value larger than the number of data points being used, the residuals becoming randomly distributed and the size distribution converging to a well behaved final form (that is to say, one that extends over more than one histogram bin, is not wildly oscillatory, and is small at either end of the diameter range). Should this occur, the easiest way to rectify it is to specify an error scaling factor that is greater than unity. An under-estimate of this factor is provided by the smallest value of $\text{SQRT}(\text{ChiSquared}/N)$ ever achieved by the program. A reasonable error scaling factor would then be, say, 1.1 times this estimate. The user should note, however, that this device should not be abused; if the rescaled errors are much larger than their true values then statistically significant information from the scattering pattern is being thrown away. Any size distribution is consistent with data of infinite errors!

CONSTANT BACKGROUND

Another likely cause of a convergence failure is an incorrect constant background subtraction. If during the previous iterations the user observed a large spike (that was not expected or predicted) at the low diameter end of the size distribution then it is quite possible that there is a constant background remaining in the data (the program is interpreting the uniform intensity as the scattering from very small particles). Conversely, if the size distribution is unreasonably biased towards large particles then it is possible that too much background has been removed and the data is missing information about the smallest particles in the sample. In either of these cases the user should specify a different amount of background. The user is reminded that of all the input parameters, the constant background subtraction is the one that needs to be known most accurately (indeed, if this parameter is inaccurate by more than about 10% then the program will probably fail). So any length of time the user spends on a precise evaluation of the constant background is probably well spent.

OTHER PARAMETERS

From a study of the size distributions plotted during the iterations the user may be able to adjust some other input parameters in order to accelerate convergence. It might, for example, be clear that the first estimate of a maximum particle diameter was too large or too small (although if it was very far out in either direction the program would have crashed rather than simply failed to converge). And it might become clear that the size distribution can be adequately described by a histogram containing fewer bins than was originally thought. Judicious removal of some particularly doubtful data points (for example those which differ in magnitude from their neighbours by an extent far greater than their errors would suggest) is also possible, though this is unlikely to have a great effect on the convergence rate.

Precisely what to do in any particular case of convergence failure depends on experience of the program which can only be gained by experimenting with it. Prospective users, once they have analyzed the BIMODAL.SAS data set are urged to re-analyze it using different combinations of diameter range, number of histogram bins, Q-vector range, aspect ratio, error scaling, and constant background (both positive and negative) to see how these variations affect the execution of the program and the final volume fraction distributions that the program produces (if it produces any). The user should then be able to recognize when and why the program is failing in any particular fitting attempt and be able to eliminate the cause.

1.4.8 AN ALTERNATE TEST DISTRIBUTION: REVERSE.SAS (by P.R. Jemian)

A new, alternate test distribution, REVERSE, has been created by P.R. Jemian to test several key questions:

#1. How close can the program get to a known volume fraction?

Note that there is no specification for the exact answer of total volume fraction for BIMODAL.SAS, only a normalized distribution [Culverwell, 1986].

#2. Does MaxSas handle data in the size range of a double-crystal instrument? #3. Do the solved distributions always look the same?

The distribution is (once again) two Gaussians in $f(D)$ space where the Gaussian at lower diameter (1100 Å, $\sigma = 300$) is 25% the height of the other Gaussian (3400 Å, $\sigma = 680$). REVERSE.DIS is the starting distribution, from which is calculated the scattering (REVERSE.SAS) using the exact form factor for spheres. An artificial volume fraction of 1.5%, artificial scattering contrast of $10.0E28 \text{ 1/m}^2$, an artificial background of 5.0 1/cm, and artificial random noise of 4% were added to the data. A summary of the analysis of the REVERSE.SAS dataset follows:

SUMMARY OF MAXSAS ANALYSIS OF REVERSE.SAS

term	analysis	actual
qMin	0.0005	—
qMax	0.025	—
NumPts	24	—
ChiSquared	23.972	—
Dmin	80	—
Dmax	8000	—
NumBins	100	—
flat entropy	4.605	—
entropy	3.925	—
Total vol. frac.	1.436%	1.5%
suggested background	4.78	5.0
vol-mean diameter	3231	3172
number-mean diameter	1181	905
error scaling factor	1.0	1.0

It appears that the spheres model can deliver the character of the correct distribution and volume fraction.

While the oscillations in the distribution suggest that there is statistical evidence for such irregular features, these cannot be believed as we know, a priori, the starting distribution and that distribution is smooth. We must conclude therefore that the entropy is not adequately maximized, subject to the constraint that ChiSquared equals the number of intensity points. While decreasing the maximum value allowed for TEST (currently set at 0.05) might seem to produce a better alignment between the entropy and ChiSquared gradients, a value as low as 0.0001 does not seem to alter the final entropy more than about 0.5%. A discussion with G.J. Daniell might bring us to resolve this point. Probably the oscillations have an origin in the introduction of the baseline “b” into the definition of the entropy as done by [Skilling, 1984]. This simplifies the math when calculating the entropy gradients but that probably makes the algorithm of [Skilling, 1984] very sensitive to gradients in the form factor.

One method to circumvent this unsightly “noise” in the solved distributions has been to replace the form factors that are defined with trig terms by ones defined by algebra. These approximations are only as good as the algebraic form can model the scattering and can render truly fictional volume fractions in the worst possible cases.

To answer, then, the three questions above, the volume fraction of the solution was very close to the actual volume fraction. The mean diameter was also very close, with the volume-weighted mean being the closest. The solved distribution was very close to the input distribution which differed dramatically in shape to the distribution of BI-MODAL.SAS, hence the solved distributions do not always look alike. The range of diameters in the distribution for REVERSE.SAS was in the range of the double-crystal instrument and so that question can be answered affirmatively. The answers are also believable and so MaxSas is not limited by the experimental range of a particular type of scattering camera.

1.4.9 SOURCE CODE

This Maximum Entropy program was originally written in BASIC by G.J. Daniell (Department of Physics, Southampton University, UK) and later translated into FORTRAN and adapted for SAS analysis by J.A. Potton. Further modifications have been made by I.D. Culverwell, G.P. Clarke and A.J. Allen (UKAEA Harwell Laboratory, UK) and P.R. Jemian (Northwestern University, USA).

There is only one source code module, MaxSas.For. Compile and link it with the fastest floating point math that you can get your hands on.

Unfortunately, some data storage had to be placed in COMMON because of the limitation of the Language Systems MPW version 1.2.1 FORTRAN compiler for the Apple Macintosh. Because of this compiler’s eccentricities, there is one compiler-dependent line of code very near the first executable statement. If you use this compiler, un-comment this line so that you get a chance to see the output. (Compiler dependence, ugh!)

As it stands on 7 February 1990, the code will now compile on:

- Digital Equipment Corporation VAX 11/785, VMS version 5.2
- Apple Macintosh, Language Systems FORTRAN v. 1.2.1
- Apple Macintosh, Microsoft (Absoft) FORTRAN v. 2.2 compiler
- MS-DOS (e.g. IBM-PC), Microsoft FORTRAN v. 5.0

Of course the program RUNS on these computers as well. Quite well!

Most of the comments in the source code have been added by P.R. Jemian. Where they exist, they are usually quite explanatory. Where they do not exist, consult the references of [Skilling, 1984] for the operation of MaxEnt.

Complete listing of MaxSas.for

```

1  PROGRAM MaxSAS
2  IMPLICIT REAL*8 (A-H,O-Z)
3  IMPLICIT INTEGER*4 (I-N)
4  CHARACTER*25 ProgVers, EditDate

```

```

5  PARAMETER ( ProgVers = '3.6 (PRJ)' )
6  PARAMETER ( EditDate = '11 February 1992' )
7  C Analysis of small-angle scattering data using the technique of
8  C entropy maximization.
9
10 C Credits:
11 C G.J. Daniell, Dept. of Physics, Southampton University, UK
12 C J.A. Potton, UKAEA Harwell Laboratory, UK
13 C I.D. Culverwell, UKAEA Harwell Laboratory, UK
14 C G.P. Clarke, UKAEA Harwell Laboratory, UK
15 C A.J. Allen, UKAEA Harwell Laboratory, UK
16 C P.R. Jemian, Northwestern University, USA
17
18 C References:
19 C 1. J Skilling and RK Bryan; MON NOT R ASTR SOC
20 C 211 (1984) 111 - 124.
21 C 2. JA Potton, GJ Daniell, and BD Rainford; Proc. Workshop
22 C Neutron Scattering Data Analysis, Rutherford
23 C Appleton Laboratory, UK, 1986; ed. MW Johnson,
24 C IOP Conference Series 81 (1986) 81 - 86, Institute
25 C of Physics, Bristol, UK.
26 C 3. ID Culverwell and GP Clarke; Ibid. 87 - 96.
27 C 4. JA Potton, GK Daniell, & BD Rainford,
28 C J APPL CRYST 21 (1988) 663 - 668.
29 C 5. JA Potton, GJ Daniell, & BD Rainford,
30 C J APPL CRYST 21 (1988) 891 - 897.
31
32 C This program was written in BASIC by GJ Daniell and later
33 C translated into FORTRAN and adapted for SANS analysis. It
34 C has been further modified by AJ Allen to allow use with a
35 C choice of particle form factors for different shapes. It
36 C was then modified by PR Jemian to allow portability between
37 C the Digital Equipment Corporation VAX and Apple Macintosh
38 C computers.
39 C The input data file format is three columns of "Q I dI" which
40 C are separated by spaces or tabs. There is no header line
41 C in the input data file.
42
43 PARAMETER (cm2m = 0.01) ! convert cm to m units, but why?
44 PARAMETER (MaxPts = 300, MaxBin = 102)
45 PARAMETER (isLin = 1, isLog = 2, ioUnit = 1)
46
47 C point-by-point mapping between reciprocal and real space
48 COMMON /space1/ grid
49 DIMENSION grid(MaxBin,MaxPts)
50
51 C terms used in entropy maximization
52 COMMON /space5/ chisq, chtarg, chizer, fSum, blank
53 COMMON /space2/ beta, c1, c2, s1, s2
54 DIMENSION beta(3), c1(3), c2(3,3), s1(3), s2(3,3)
55
56 C terms used only by subroutine MaxEnt, allocated here to make memory tidy
57 COMMON /space3/ ox, z, cgrad, sgrad, xi, eta
58 DIMENSION ox(MaxPts), z(MaxPts)
59 DIMENSION cgrad(MaxBin), sgrad(MaxBin)
60 DIMENSION xi(MaxBin,3), eta(MaxPts,3)
61
62 C space for the plotting frame, allocated here to make memory tidy

```

```

63 C   note the limits: MaxCol <= 100, MaxRow <= 150 (really large screens!)
64   PARAMETER (MaxCol = 75, MaxRow = 15)
65   PARAMETER (MxC2 = MaxCol+2, MxR2 = MaxRow+2)
66   COMMON /space4/ screen, nCol, nRow, nCol2, nRow2
67   CHARACTER*1 screen(100, 150)
68
69 C   space for main segment arrays
70   DIMENSION q(MaxPts), datum(MaxPts), sigma(MaxPts)
71   DIMENSION r(MaxBin), f(MaxBin), base(MaxBin), Qty(MaxBin)
72   DIMENSION fit(MaxPts), BinWid(MaxBin)
73   DIMENSION SkyFit(MaxPts), SkyDis(MaxBin)
74   CHARACTER*40 InFile, OutFil
75   LOGICAL Yes
76   CHARACTER*1 YN, aTab
77
78   DATA one, zero /1.0, 0.0/   ! compiler-independence!
79   DATA hrDamp /5.0/           ! model 7&8: sets transition range
80   DATA htDamp /0.9/          ! model 7: amount of damping
81 C   The value "hrDamp" sets the range where the transition occurs.
82 C   The value "htDamp" sets the maximum proportion of damping.
83
84 C   ... Define (initially) the default responses
85   DATA iOption /4/           ! usual form factor for spheres
86   DATA Aspect /1.0/          ! particle aspect ratio
87   DATA LinLog /isLin/        ! linear binning scale
88   DATA n /40/                ! number of bins
89   DATA Dmin, Dmax /8.00, 400.0/ ! particle diameters
90   DATA IterMax /20/          ! maximum number of iterations to try
91   DATA RhoSq /1.0/           ! scattering contrast, x10**28 1/m**4
92   DATA fac, err /1.0, 1.0/   ! scalars for intensity and errors
93   DATA qMin, qMax /1.e-8, 100./ ! range to accept
94   DATA Bkg /0.0/             ! intensity to subtract
95   DATA sLengt /1.0E-20/      ! rectangular slit-length, 1/A
96   DATA SkyBkg /1.0E-6/       ! the so-called "sky background" of [1]
97
98 C   Next line for MPW/Language Systems version 1.2.1, Macintosh only
99 C   Comment this out for other compilers
100 C   This is the only compiler-dependent line in this source code!!!!!!
101 C   CALL OutWindowScroll (1000) ! for 1-line advance screen
102
103   pi = 4. * ATAN(1.)
104   aTab = CHAR (9)
105
106 C   screen dimension variables for plots, in COMMON /space4/
107   nCol = MaxCol
108   nRow = MaxRow
109   nCol2 = MxC2
110   nRow2 = MxR2
111
112   1  WRITE (*,*)
113   WRITE (*,*) 'Size distributions from SAS data using the',
114   >           ' maximum entropy criterion'
115   WRITE (*,*) '      version: ', ProgVers
116   WRITE (*,*) '  Last edited: ', EditDate
117
118   CALL GetInf (InFile, OutFil, iOption, Aspect, LinLog,
119   >           n, Dmin, Dmax, IterMax, RhoSq, fac, err, qMin,
120   >           qMax, Bkg, sLengt, SkyBkg, hrDamp, htDamp)

```

```

121 IF (InFile .EQ. ' ') STOP
122
123 C Read in the SAS data from the file "InFile"
124 WRITE (*,*) ' Reading from file: ', InFile
125 OPEN (UNIT = ioUnit, FILE = InFile, STATUS = 'old')
126 DO j = 1, MaxPts
127 READ (ioUnit, *, END = 95) q(j), datum(j), sigma(j)
128 END DO
129 95 npt=j-1 ! ignore any lines without an explicit EOL mark
130 CLOSE (UNIT = ioUnit, STATUS = 'keep')
131 WRITE (*,*) npt, ' points were read from the file'
132
133 C Subtract background, convert to 1/m units and
134 C shift for the selected data range
135 i = 0
136 DO j = 1, npt
137 IF (q(j) .GE. Qmin .AND. q(j) .LE. Qmax) THEN
138 i = i + 1
139 q(i) = q(j)
140 datum(i) = fac * (datum(j)-Bkg) / cm2m
141 sigma(i) = fac * err * sigma(j) / cm2m
142 END IF
143 END DO
144 npt = i
145 WRITE (*,*) npt, ' points were selected from the data'
146
147 C PRJ: 24 May 1989
148 C BinWid: actual radial width of the indexed bin number
149 C Step: radial increment factor (for geometric series)
150 C rWid: radial width (for arithmetic series)
151 IF (LinLog .EQ. isLog) THEN ! geometric series
152 Step = (Dmax/Dmin)**(1. / FLOAT(n-1)) - 1.
153 rWid = 0.
154 ELSE ! arithmetic series
155 Step = 0.
156 rWid = 0.5*(Dmax - Dmin) / FLOAT(n-1)
157 END IF
158 r(1) = 0.5 * Dmin
159 BinWid(1) = r(1) * Step + rWid
160 DO i = 2, n
161 r(i) = r(i-1) + BinWid(i-1)
162 BinWid(i) = r(i) * Step + rWid
163 END DO
164
165 WRITE (*,*) ' Preparation of the GRID function...'
166 C Calculate the form-factor pre-terms
167 111 IF (iOption .EQ. 1) THEN ! Rods, using model of AJ Allen
168 alphan1 = 2. * pi * Aspect
169 alphan2 = 4. * pi
170 preform = alphan1
171 sLengt = 0. ! "pinhole" collimation
172 ELSE IF (iOption .EQ. 2) THEN ! Disks, using model of AJ Allen
173 alphan1 = 2. * pi / (Aspect**2)
174 alphan2 = 2. * pi
175 preform = alphan1
176 sLengt = zero
177 ELSE IF (iOption .EQ. 3) THEN ! Globules, using model of AJ Allen
178 alphan1 = 4. * pi * Aspect / 3.

```

```

179 IF (Aspect .LT. 0.99) THEN      ! hamburger-shaped
180   sqqt = SQRT (one - Aspect**2)
181   argument = (2. - Aspect**2 + 2. * sqqt) / (Aspect**2)
182   surchi = (one + Aspect**2 * LOG(argument) / (2.*sqqt) )
183   >   / ((2. * Aspect))
184 ELSE IF (Aspect .GT. 1.01) THEN  ! peanut shaped
185   sqqt = SQRT(Aspect**2 - one)
186   argument = sqqt / Aspect
187   surchi = (one + Aspect**2 * ASIN(argument) / sqqt)
188   >   / ((2. * Aspect))
189 ELSE                               ! spheroidal
190   surchi = one
191 END IF
192 alphan2 = 6. * pi * surchi
193 preform = alphan1
194 sLengt = zero
195 ELSE IF (iOption .EQ. 4) THEN      ! Spheres, delta-function
196   alphan1 = 4. * pi / 3.
197   alphan2 = 6. * pi
198   preform = 9. * alphan1
199   sLengt = zero
200 ELSE IF (iOption .EQ. 5) THEN      ! Spheres, box-distribution
201   alphan1 = 4. * pi / 3.          ! This model by PRJ
202   alphan2 = 6. * pi
203   preform = 48. * pi
204   sLengt = zero
205 ELSE IF (iOption .EQ. 6) THEN      ! smeared, spheroidal globs
206   preform = 4. * Pi / 3.          ! This model by PRJ
207   alphan1 = preform
208   alphan2 = 6. * Pi
209   Cgs = SQRT (3. * Pi)           ! for low-Q region
210   Cps = 9. * Pi / 4.             ! for med. high-Q region
211   Cp = 9. / 2.                   ! for high-Q region
212 ELSE IF (iOption .EQ. 7) THEN      ! spheroidal globs, no smearing
213   preform = 4. * Pi / 3.          ! This model by PRJ
214   alphan1 = preform
215   alphan2 = 6. * Pi
216   sLengt = zero
217 ELSE IF (iOption .EQ. 8) THEN      ! smooth spheres
218   preform = 4. * Pi / 3.          ! This model by PRJ
219   alphan1 = preform
220   alphan2 = 6. * Pi
221   sLengt = zero
222 END IF
223
224 C alphaN1 is RhoSq * the particle volume
225 C alphaN2 is RhoSq * the particle surface area / the particle volume
226 C ... and later divided by q**4
227   alphan1 = cm2m * alphan1 * rhosq * r(1)**3
228   alphan2 = cm2m * alphan2 * rhosq / r(n)
229   preform = cm2m * preform * rhosq
230
231 DO   i = 1, n
232   rCubed = r(i)**3
233   DO   j = 1, npt
234     Qr = q(j) * r(i)
235     Qr2 = Qr**2
236     IF (iOption .EQ. 1) THEN

```

```

237     QH = q(j) * Aspect * r(i)      ! rod 1/2 - length
238     topp = one + 2.*Pi* QH**3 * Qr / (9 * (4 + Qr**2))
239 >     + (QH**3 * Qr**4) / 8.
240     bott = one + QH**2 * (one + QH**2 * Qr)/9
241 >     + (QH**4 * Qr**7) / 16
242     ELSE IF (iOption .EQ. 2) THEN
243     h = r(i)      ! disk 1/2 - thickness
244     Rd = h / Aspect      ! disk radius
245     Qh = q(j) * h
246     QRd = q(j) * Rd
247     topp = one + QRd**3 / (3. + Qh**2)
248 >     + (Qh**2 * QRd / 3.)**2
249     bott = one + QRd**2 * (one + Qh * QRd**2) / 16
250 >     + (Qh**3 * QRd**2 / 3.)**2
251     ELSE IF (iOption .EQ. 3) THEN
252     topp = one
253     bott = one + Qr**2 * (2. + Aspect**2) / 15.
254 >     + 2. * Aspect * Qr**4 / (9. * surchi)
255     ELSE IF (iOption .EQ. 4) THEN
256     topp = (SIN(Qr) - Qr * COS(Qr))**2
257     bott = Qr**6
258     ELSE IF (iOption .EQ. 5) THEN
259     Qj = q(j)
260     rP = r(i) + BinWid(i)
261     rM = r(i)
262     bP = 0.5*rP + (Qj**2)*(rP**3)/6.
263 >     + (0.25*(Qj * rP**2) - 0.625/Qj) * SIN (2.*Qj*rP)
264 >     + 0.75 * rP * COS (2.*Qj*rP)
265     bM = 0.5*rM + (Qj**2)*(rM**3)/6.
266 >     + (0.25*(Qj * rM**2) - 0.625/Qj) * SIN (2.*Qj*rM)
267 >     + 0.75 * rM * COS (2.*Qj*rM)
268     topp = bP - bM
269     bott = Qj**6 * (rP**4 - rM**4) * rCubed
270     ELSE IF (iOption .EQ. 6) THEN
271     rL = r(i) * sLengt
272     topp = Cgs
273     bott = rL*(one + Qr2/5. + Cgs/Cps * Qr**3)
274 >     + Cgs/Cp * Qr**4
275     ELSE IF (iOption .EQ. 7) THEN
276 C The value "hrDamp" sets the range where the transistion occurs.
277 C The value "htDamp" sets the maximum proportion of damping.
278 C The weight is a "step" function with a broad edge.
279     weight = htDamp * EXP (-Qr2/hrDamp**2) + (one - htDamp)
280     topp = 3. * (SIN(Qr) - Qr * COS(Qr)) / Qr**3
281     bott = 4.5 / Qr**4      ! bott=<topp**2> for large Qr
282     topp = weight * topp**2 + (one-weight) / (one + one/bott)
283     bott = one
284     ELSE IF (iOption .EQ. 8) THEN ! like #7 but smoother
285     Qr2 = Qr**2
286     weight = EXP (-Qr2/hrDamp**2)
287     IF (Qr .LE. Pi) THEN
288     topp = ((-1./45360.*Qr2+1./840.)*Qr2-1./30.)*Qr2+1./3.
289     ELSE
290     topp = 0.0
291     END IF
292     topp = (3*topp)**2
293     bott = 4.5 / Qr**4
294     topp = weight*topp + (1-weight)/(1 + 1/bott)

```

```

295     bott = one
296     END IF
297     grid(i,j) = preform * rCubed * topp / bott
298 C     factors of 4Pi/3 are already included in "preform"
299     END DO
300     END DO
301
302 C     Attempt to account for scattering from very large and very small
303 C     particles by use of the limiting forms of grid(i,j).
304     DO j = 1, npt
305         grid(n+1,j) = alphan1 ! next line accounts for a slit-length
306         grid(n+2,j) = alphan2 / (q(j)**3 * SQRT(q(j)**2 + sLengt**2))
307     END DO
308
309 C     Try to solve the problem
310 C     228 basis = 1.0e-6 / RhoSq ! Originally was just 1.0e-6
311     basis = SkyBkg ! PRJ, 18.6.90
312     228 CALL MaxEnt (n+2,npt, f,datum,sigma, basis,base, max,itermax)
313
314 C     "Max" counts the number of iterations inside MAXENT.
315 C     If Max < IterMax, then the problem has been solved.
316     IF (max .GE. itermax) THEN
317         WRITE (*,*) ' No convergence! # iter. = ', max
318         WRITE (*,*) ' File was: ', InFile
319         GO TO 1
320     END IF
321
322 C     Otherwise, SUCCESS!... so calculate the SAS from the distribution
323     CALL opus (n+2, npt, f, fit)
324     CALL opus (n+2, npt, base, SkyFit) ! fit the sky background, too!
325
326 C     ... and remove the bin width effect.
327 C     Also, calculate the total volume fraction, the mode, mean, and
328 C     standard deviations of the volume and number distributions.
329     SumV = zero
330     SumVR = zero
331     SumVR2 = zero
332     SumN = zero
333     SumNR = zero
334     SumNR2 = zero
335     modeV = 1
336     modeN = 1
337     DO i = 1, n
338         size = r(i)
339         frac = f(i)
340         pVol = 4*Pi/3 * (size * 1.e-8)**3 ! particle volume, cm**3
341         IF (iOption .EQ. 1) pVol = pVol * Aspect ! rods
342         IF (iOption .EQ. 2) pVol = pVol / Aspect ! disks
343         IF (iOption .EQ. 3) pVol = pVol * Aspect ! globs
344         amount = (frac - SkyBkg) / pVol ! number / cm**3
345         IF (amount .LT. zero) amount = zero
346         f(i) = frac / BinWid(i)
347         base(i) = base(i) / BinWid(i)
348         Qty(i) = amount / BinWid(i)
349         IF (i .GT. 3) THEN ! ignore 1st few bins
350             SumN = SumN + amount
351             SumNR = SumNR + amount * size
352             SumNR2 = SumNR2 + amount * size**2

```

```

353     END IF
354     IF (Qty(i) .GT. Qty(modeN)) modeN = i ! get the mode
355     SumV   = SumV   + frac
356     SumVR  = SumVR  + frac * size
357     SumVR2 = SumVR2 + frac * size**2
358     IF (f(i) .GT. f(modeV)) modeV = i      ! get the mode
359     END DO
360     DnMean = 2.0 * SumNR / SumN
361     DnSDev = 2.0 * SQRT((SumNR2 / SumN) - (SumNR / SumN)**2)
362     DvMean = 2.0 * SumVR / SumV
363     DvSDev = 2.0 * SQRT((SumVR2 / SumV) - (SumVR / SumV)**2)
364
365     Entropy = zero
366     DO i = 1, n
367         frac = BinWid(i) * f(i) / SumV      ! Skilling & Bryan, eq. 1
368         Entropy = Entropy - frac * LOG (frac)
369     END DO
370
371 C Show the final distribution, corrected for bin width.
372
373     WRITE (*,*)
374     WRITE (*,*) ' Input file: ', InFile
375     WRITE (*,*) ' Volume weighted size dist.: V(r)N(r) versus r'
376     CALL Plot (n, r, f)
377
378 C Estimate a residual background that remains in the data.
379     Sum1 = zero
380     Sum2 = zero
381     DO j = 1, npt
382         weight = one / (sigma(j)**2)
383         Sum1 = Sum1 + weight * (fit(j) - datum(j))
384         Sum2 = Sum2 + weight
385     END DO
386     shift = Sum1 / Sum2
387
388 C Scale the data back to 1/cm units and calculate Chi-squared
389     ChiSq = zero
390     Chi2Bk = zero
391     DO j = 1, npt
392         z(j) = (datum(j) - fit(j)) / sigma(j)
393         ChiSq = ChiSq + z(j)**2
394         Chi2Bk = Chi2Bk + (z(j) + shift/ sigma(j))**2
395         datum(j) = cm2m * datum(j)
396         sigma(j) = cm2m * sigma(j)
397         fit(j) = cm2m * fit(j)
398         SkyFit(j) = cm2m * SkyFit(j)
399     END DO
400     shift = cm2m * shift / fac
401
402     WRITE (*,*) ' standardized residuals vs. point number'
403     CALL ResPlt (npt, z)
404
405 C Let the file output begin!
406
407     OPEN (UNIT = ioUnit, FILE=OutFil, STATUS='new')
408     WRITE (ioUnit,*) ' Results of maximum entropy analysis of SAS'
409     WRITE (ioUnit,*) '      version: ', aTab, ProgVers
410     WRITE (ioUnit,*) '      edited: ', aTab, EditDate

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411 WRITE (ioUnit,*)
412 WRITE (ioUnit,*) ' input file: ', aTab, InFile
413 WRITE (ioUnit,*) ' output file: ', aTab, OutFil
414 WRITE (ioUnit,*)
415 WRITE (ioUnit, 35591) 'D, A', aTab, 'f, 1/A',
416 > aTab, 'Bkg f, 1/A', aTab, 'N dD, 1/A/cm^3'
417 35591 FORMAT (1X, A12, 3(A1, 1X, A15))
418
419 DO i = 1, n
420 WRITE (ioUnit,3559) 2.*r(i), aTab, 0.5*f(i), aTab,
421 > 0.5*Base(i), aTab, 0.5*Qty(i)
422 END DO
423 3559 FORMAT (1X, F12.2, 3(A1, 1X, 1PE15.5))
424
425
426 WRITE (ioUnit, 1011) 'Q 1/A', aTab, 'I 1/cm', aTab,
427 > 'fit I 1/cm', aTab, 'dI 1/cm', aTab,
428 > 'SkyFit 1/cm', aTab, 'z'
429 1011 FORMAT (///, A12, 5(1X, A1, A12))
430
431 DO j = 1, npt
432 WRITE (ioUnit,560) q(j), aTab, datum(j), aTab, fit(j),
433 > aTab, sigma(j), aTab, SkyFit(j), aTab, z(j)
434 END DO
435 560 FORMAT (1PE12.4, 4(A1, E13.5), 1X, A1, OPF12.6)
436
437 WRITE (ioUnit,3301) aTab, InFile
438 WRITE (*,3301) aTab, InFile
439 3301 FORMAT (//' Input data: ', A1, A40)
440
441 WRITE (ioUnit,3302) RhoSq
442 WRITE (*,3302) RhoSq
443 3302 FORMAT (' Contrast = ', F15.7, ' x 10^28 m^-4.')
444
445 IF (iOption .EQ. 1) THEN
446 WRITE (ioUnit,*) ' rods: dia=D, length=D*', Aspect
447 WRITE (*,*) ' rods: dia=D, length=D*', Aspect
448 ELSE IF (iOption .EQ. 2) THEN
449 WRITE (ioUnit,*) ' disks: thickness=D, dia=D/', Aspect
450 WRITE (*,*) ' disks: thickness=D, dia=D/', Aspect
451 ELSE IF (iOption .EQ. 3) THEN
452 WRITE (ioUnit,*) ' globs: D x D x D*', Aspect
453 WRITE (*,*) ' globs: D x D x D*', Aspect
454 ELSE IF (iOption .EQ. 4) THEN
455 WRITE (ioUnit,*) ' delta-function Spheres: diameter=D'
456 WRITE (*,*) ' delta-function Spheres: diameter=D'
457 ELSE IF (iOption .EQ. 5) THEN
458 WRITE (ioUnit,*) ' box-function Spheres: diameter=D'
459 WRITE (*,*) ' box-function Spheres: diameter=D'
460 ELSE IF (iOption .EQ. 6) THEN
461 WRITE (ioUnit,*) ' slit-smearred spheroidal globs: diameter=D'
462 WRITE (*,*) ' slit-smearred spheroidal globs: diameter=D'
463 WRITE (ioUnit,*) ' slit-length (1/A) = ', sLengt
464 WRITE (*,*) ' slit-length (1/A) = ', sLengt
465 ELSE IF (iOption .EQ. 7) THEN
466 WRITE (ioUnit,*) ' spheroidal globs: diameter=D'
467 WRITE (*,*) ' spheroidal globs: diameter=D'
468 ELSE IF (iOption .EQ. 8) THEN

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469     WRITE (ioUnit,*) ' smooth spheres: diameter=D'
470     WRITE (*,*) ' smooth spheres: diameter=D'
471 END IF
472
473     WRITE (ioUnit,53303) fac
474     WRITE (*,53303) fac
475 53303   FORMAT (' Data conversion factor to 1/cm = ', 1PE12.5)
476
477     WRITE (ioUnit,63303) err
478     WRITE (*,63303) err
479 63303   FORMAT (' Error scaling factor = ', 1PE12.5)
480
481     IF (LinLog .EQ. isLog) THEN
482         WRITE (ioUnit,13304) 'geometric'
483         WRITE (*,13304) 'geometric'
484     ELSE
485         WRITE (ioUnit,13304) 'arithmetic'
486         WRITE (*,13304) 'arithmetic'
487     END IF
488 13304   FORMAT (' Histogram bins are distributed in an increasing ',
489 >           A10, ' series.')
490
491     WRITE (ioUnit,3304) 'Minimum', Dmin
492     WRITE (*,3304) 'Minimum', Dmin
493     WRITE (ioUnit,3304) 'Maximum', Dmax
494     WRITE (*,3304) 'Maximum', Dmax
495 3304   FORMAT (1X, A7, ' particle dimension D = ',F12.2,' A.')
496
497     WRITE (ioUnit,3306) n
498     WRITE (*,3306) n
499 3306   FORMAT (' Number of histogram bins = ',I4,'.')
500
501     WRITE (ioUnit,3307) itermax
502     WRITE (*,3307) itermax
503 3307   FORMAT (' Maximum number of iterations allowed = ',I4,'.')
504
505     WRITE (ioUnit,3314) max
506     WRITE (*,3314) max
507 3314   FORMAT (' Program left MaxEnt routine after ',
508 *           I4,' iterations.')
509
510     WRITE (ioUnit,3308) npt
511     WRITE (*,3308) npt
512 3308   FORMAT (' Target chi-squared (# data points) = ',I5,'.')
513
514     WRITE (ioUnit,3309) ChiSq
515     WRITE (*,3309) ChiSq
516 3309   FORMAT (' Best value of chi-squared achieved = ',F12.6,'.')
517
518     WRITE (ioUnit, 33091) 'the final', Entropy
519     WRITE (*, 33091) 'the final', Entropy
520     WRITE (ioUnit, 33091) 'a flat', LOG (FLOAT (n))
521     WRITE (*, 33091) 'a flat', LOG (FLOAT (n))
522 33091   FORMAT (' Entropy of ', A9, ' distribution = ', F12.7,'.')
523
524     WRITE (ioUnit,33101) SumN
525     WRITE (*,33101) SumN
526 33101   FORMAT (' Total particles = ', 1PE15.5,' per cubic cm.')

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527
528 WRITE (ioUnit,3310) SumV
529 WRITE (*,3310) SumV
530 3310 FORMAT (' Total volume fraction of all scatterers = ',
531 * F15.9, '.')
532
533 WRITE (ioUnit,3311) 'smaller', Dmin, f(n+1)
534 WRITE (ioUnit,3311) 'larger', Dmax, f(n+2)
535 WRITE (*,3311) 'smaller', Dmin, f(n+1)
536 WRITE (*,3311) 'larger', Dmax, f(n+2)
537 3311 FORMAT (' Volume fraction ',A7,' than ', F12.2,
538 * ' A = ', 1PE13.5, '.')
539
540 WRITE (ioUnit,3411) SkyBkg
541 WRITE (*,3411) SkyBkg
542 3411 FORMAT (' Sky background (minimum ',
543 * ' significant volume fraction) = ', 1PE13.5, '.')
544
545 WRITE (ioUnit,3312) 'Volume', 'mode D value', 2.0 * r(modeV)
546 WRITE (*,3312) 'Volume', 'mode D value', 2.0 * r(modeV)
547 WRITE (ioUnit,3312) 'Volume', 'mean D value', DvMean
548 WRITE (*,3312) 'Volume', 'mean D value', DvMean
549 WRITE (ioUnit,3312) 'Volume', 'std. deviation', DvSDev
550 WRITE (*,3312) 'Volume', 'std. deviation', DvSDev
551 WRITE (ioUnit,3312) 'Number', 'mode D value', 2.0 * r(modeN)
552 WRITE (*,3312) 'Number', 'mode D value', 2.0 * r(modeN)
553 WRITE (ioUnit,3312) 'Number', 'mean D value', DnMean
554 WRITE (*,3312) 'Number', 'mean D value', DnMean
555 WRITE (ioUnit,3312) 'Number', 'std. deviation', DnSDev
556 WRITE (*,3312) 'Number', 'std. deviation', DnSDev
557 3312 FORMAT (1X, A6, '-weighted ', A14, ' = ', F12.5, ' A.')
558
559 WRITE (ioUnit,3313) 'Min', q(1)
560 WRITE (*,3313) 'Min', q(1)
561 WRITE (ioUnit,3313) 'Max', q(npt)
562 WRITE (*,3313) 'Max', q(npt)
563 3313 FORMAT (1X, A3, 'imum Q-vector = ', 1PE15.7, ' 1/A.')
564
565 WRITE (ioUnit,3315) 'User-specified', Bkg
566 WRITE (*,3315) 'User-specified', Bkg
567 WRITE (ioUnit,3315) 'Suggested', Bkg - shift
568 WRITE (*,3315) 'Suggested', Bkg - shift
569 3315 FORMAT (1X, A14, ' background = ', F18.9, ' input data units')
570
571 WRITE (ioUnit,*) ' New background should give ChiSq = ', Chi2Bk
572 WRITE (*,*) ' New background should give ChiSq = ', Chi2Bk
573
574 CLOSE (UNIT=ioUnit, STATUS='keep')
575
576 C Adjust the background default setting
577 C Shift the intensity data just in case the user wants a Stability Check
578 C Remember: background shifts down, intensity shifts up
579 C Don't forget to put the data back into units of 1/m!
580 Bkg = Bkg - shift
581 DO j = 1, npt
582 datum(j) = (datum(j) + shift) / cm2m
583 sigma(j) = sigma(j) / cm2m
584 END DO

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585
586     IF (ABS ((Chi2Bk-ChiSq)/FLOAT (npt)) .LE. 0.05) THEN
587         WRITE (*,*) ' The change in ChiSquared should be < 5%.'
588 4000     WRITE (*, '(X,A,$)') ' Run the Stability Check? (Y/<N>)'
589         READ (*, '(A1)') YN
590         IF (YN .EQ. 'y' .OR. YN .EQ. 'Y') GO TO 228
591         IF (YN .NE. ' ' .AND. YN .NE. 'n' .AND. YN .NE. 'N') GO TO 4000
592     END IF
593
594     WRITE (*,3200) OutFil
595 3200     FORMAT (/,' The program is finished.', /,
596         1     ' The output file is: ', A40)
597     GO TO 1
598
599 3199     STOP
600     END
601
602
603     SUBROUTINE GetInf (InFile, OutFil, iOption, Aspect, LinLog,
604         >         nBin, Dmin, Dmax, IterMax, RhoSq, fac, err, qMin,
605         >         qMax, Bkg, sLengt, SkyBkg, hrDamp, htDamp)
606     IMPLICIT REAL*8 (A-H,O-Z)
607     IMPLICIT INTEGER*4 (I-N)
608     CHARACTER*40 InFile, OutFil
609     PARAMETER (Ro2Max = 1.e6, ItrLim = 200, AbsMax = 1.e3)
610     PARAMETER (DiaMin = 1., DiaMax = 1.e6, ErrMax = 1.e6)
611     PARAMETER (MaxPts = 300, MaxBin = 102)
612     PARAMETER (isLin = 1, isLog = 2)
613
614     1     WRITE (*, '(X,A,$)') ' Input file? <Quit>'
615         READ (*, 2) InFile
616     2     FORMAT (A40)
617         IF (InFile.EQ.' ') RETURN
618
619     3     WRITE (*, '(X,A,$)') ' Output file?'
620         READ (*, 2) OutFil
621         IF (OutFil .EQ. ' ') GO TO 3
622         IF (OutFil .EQ. InFile) GO TO 1
623
624     suggest = qMin
625 16     WRITE (*, '(X,A,G,A,$)') ' Minimum q-vector? [1/A] <',
626         >         suggest, '>'
627         READ (*, '(F10.0)') qMin
628         IF (qMin .LT. 0) GO TO 16
629         IF (qMin .EQ. 0) qMin = suggest
630
631     suggest = qMax
632 17     WRITE (*, '(X,A,G,A,$)') ' Maximum q-vector? [1/A] <',
633         >         suggest, '>'
634         READ (*, '(F10.0)') qMax
635         IF (qMax .EQ. 0) qMax = suggest
636         IF (qMax .LE. 0) GO TO 17
637         IF (qMax .LE. qMin) GO TO 1
638
639     suggest = RhoSq
640 13     WRITE (*, '(X,A,G,A,$)')
641         >         ' Scattering contrast? [10^28 m^-4] <', suggest, '>'
642         READ (*, '(F10.0)') RhoSq

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643 IF (RhoSq .EQ. 0) RhoSq = suggest
644 IF (RhoSq .LT. 0 .OR. RhoSq .GT. Ro2Max) GO TO 13
645
646 suggest = fac
647 14 WRITE (*, '(X,A,G,A,$)')
648 > ' Factor to convert data to 1/cm? <', suggest, '>'
649 READ (*, '(F10.0)') fac
650 IF (fac .EQ. 0) fac = suggest
651 IF (fac .LE. 0 .OR. fac .GT. AbsMax) GO TO 14
652
653 suggest = err
654 15 WRITE (*, '(X,A,G,A,$)')
655 > ' Error scaling factor? <', suggest, '>'
656 READ (*, '(F10.0)') err
657 IF (err .EQ. 0) err = suggest
658 IF (err .LE. 0 .OR. err .GT. ErrMax) GO TO 15
659
660 suggest = Bkg
661 18 WRITE (*, '(X,A,G,A,$)') ' Background? <', suggest, '>'
662 READ (*, '(F10.0)') Bkg
663 IF (Bkg .EQ. 0) Bkg = suggest
664
665 Last = iOption
666 4 WRITE (*,*) ' Select a form model for the scatterer:'
667 WRITE (*,*) ' (See the User Guide for complete explanations)'
668 WRITE (*,*) ' 1: rods          2: disks          3: globules'
669 WRITE (*,*) ' 4: spheres (usual form)          ',
670 > '5: spheres (integrated)'
671 WRITE (*,*) ' 6: spheroids (slit-smear)          ',
672 > '7: spheroidal globs (not smeared)'
673 WRITE (*,*) ' 8: smoothed spheres (not smeared)'
674 WRITE (*, '(X,A,I3,A,$)')
675 > ' Which option number? <', Last, '>'
676 READ (*, '(I4)') iOption
677 IF (iOption .EQ. 0) iOption = Last
678 IF (iOption .LT. 1 .OR. iOption .GT. 8) GO TO 4
679
680 suggest = Aspect
681 6 IF (iOption .GE. 1 .AND. iOption .LE. 3) THEN
682 WRITE (*,*) ' AR = Aspect Ratio, useful ranges are indicated'
683 IF (iOption .EQ. 1) THEN
684 WRITE (*,*) ' diameter D, length D * AR, AR > 5'
685 ELSE IF (iOption .EQ. 2) THEN
686 WRITE (*,*) ' thickness D, diameter D / AR, AR < 0.2'
687 ELSE IF (iOption .EQ. 3) THEN
688 WRITE (*,*) ' D x D x D * AR, 0.3 < AR < 3'
689 END IF
690 WRITE (*, '(X,A,G,A,$)')
691 > ' Aspect ratio? <', suggest, '>'
692 READ (*, '(F10.0)') Aspect
693 IF (Aspect .EQ. 0) Aspect = suggest
694 IF (Aspect .LT. 0) GO TO 6
695 END IF
696
697 suggest = sLengt
698 61 IF (iOption .EQ. 6) THEN
699 WRITE (*, '(X,A,G,A,$)')
700 > ' Slit-smear'd globs. Slit-length [1/A]? <',

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```

701     > suggest, '>'
702     READ (*, '(F10.0)') sLengt
703     IF (sLengt .EQ. 0) sLengt = suggest
704     IF (sLengt .LT. 0) GO TO 61
705     END IF
706
707     suggest = htDamp
708 62 IF (iOption .EQ. 7) THEN
709     WRITE (*, '(X,A,G,A,$)')
710     > ' spheroidal globs. fraction of standard function? <',
711     > suggest, '>'
712     READ (*, '(F10.0)') htDamp
713     IF (htDamp .EQ. 0) htDamp = suggest
714     IF (htDamp .LT. 0) GO TO 62
715     IF (htDamp .GT. 1) GO TO 62
716     END IF
717
718     suggest = hrDamp
719 63 IF (iOption .EQ. 7 .OR. iOption .EQ. 8) THEN
720     WRITE (*, '(X,A,G,A,$)')
721     > ' smoothed spheres. Onset Qr value? <',
722     > suggest, '>'
723     READ (*, '(F10.0)') hrDamp
724     IF (hrDamp .EQ. 0) hrDamp = suggest
725     IF (hrDamp .LT. 0) GO TO 63
726     END IF
727
728     Last = LinLog
729     7 WRITE (*, '(X,A,I2,A,$)')
730     > ' Bin step scale? (1=Linear, 2=Log) <', Last, '>'
731     READ (*, '(I4)') LinLog
732     IF (LinLog .EQ. 0) LinLog = Last
733     IF (LinLog .NE. isLin .AND. LinLog .NE. isLog) GO TO 7
734
735     Last = nBin
736     8 WRITE (*, '(X,A,I4,A,$)')
737     > ' Number of histogram bins? <', Last, '>'
738     READ (*, '(I4)') nBin
739     IF (nBin .EQ. 0) nBin = Last
740     IF (nBin .LT. 2 .OR. nBin .GT. (MaxBin-2)) GO TO 8
741
742     suggest = Dmax
743     9 WRITE (*, '(X,A,G,A,$)')
744     > ' Maximum value of D? [A] <', suggest, '>'
745     READ (*, '(F10.0)') Dmax
746     IF (Dmax .EQ. 0) Dmax = suggest
747     IF (Dmax .LT. nBin*DiaMin .OR. Dmax .GE. DiaMax) GO TO 9
748
749     Suggest = Dmax / FLOAT (nBin)
750 11 WRITE (*, '(X,A,G,A,$)')
751     > ' Minimum value of D? [A] <', suggest, '>'
752     READ (*, '(F10.0)') Dmin
753     IF (Dmin .EQ. 0) Dmin = suggest
754     IF (Dmin .GE. DMax .OR. Dmin .LT. DiaMin) GO TO 1
755
756     IF (IterMax .GT. ItrLim) IterMax = ItrLim
757     Last = IterMax
758 12 WRITE (*, '(X,A,I4,A,$)')

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```

759     >      ' Maximum number of iterations? <', Last, '>'
760 READ (*, '(I4)') IterMax
761 IF (IterMax .EQ. 0) IterMax = Last
762 IF (IterMax .LT. 0 .OR. IterMax .GT. ItrLim) GO TO 12
763
764 Suggest = SkyBkg
765 21      WRITE (*, '(X,A,G,A,$)')
766     >      ' Sky background? (positive) <', Suggest, '>'
767 READ (*, '(F10.0)') SkyBkg
768 IF (SkyBkg .LT. 0) GO TO 21
769 IF (SkyBkg .EQ. 0) SkyBkg = Suggest ! keep default
770
771 RETURN
772 END
773
774
775 SUBROUTINE opus(n,npt,x,ox) ! solution-space -> data-space
776 IMPLICIT REAL*8 (A-H,O-Z)
777 IMPLICIT INTEGER*4 (I-N)
778 PARAMETER (MaxPts=300, MaxBin=102)
779 COMMON /spacel/ grid
780 DIMENSION x(MaxBin), grid(MaxBin,MaxPts), ox(MaxPts)
781 DO   j = 1, npt
782     sum = 0.
783     DO   i = 1, n
784         sum = sum + x(i) * grid(i,j)
785     END DO
786     ox(j) = sum
787 END DO
788 RETURN
789 END
790
791
792 SUBROUTINE tropus(n,npt,ox,x) ! data-space -> solution-space
793 IMPLICIT REAL*8 (A-H,O-Z)
794 IMPLICIT INTEGER*4 (I-N)
795 PARAMETER (MaxPts=300, MaxBin=102)
796 COMMON /spacel/ grid
797 DIMENSION x(MaxBin), grid(MaxBin,MaxPts), ox(MaxPts)
798 DO   i = 1, n
799     sum = 0.
800     DO   j = 1, npt
801         sum = sum + ox(j) * grid(i,j)
802     END DO
803     x(i) = sum
804 END DO
805 RETURN
806 END
807
808
809 SUBROUTINE MaxEnt(n,npt, f,datum,sigma, flat,base,iter,itermax)
810 IMPLICIT REAL*8 (A-H,O-Z)
811 IMPLICIT INTEGER*4 (I-N)
812 PARAMETER (MaxPts=300, MaxBin=102)
813 DIMENSION f(MaxBin), datum(MaxPts), sigma(MaxPts)
814 DIMENSION base(MaxBin)
815
816 COMMON /spacel/ grid

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```

817 DIMENSION grid(MaxBin,MaxPts)
818
819 COMMON /space5/ chisq, chtarg, chizer, fSum, blank
820 COMMON /space2/ beta, c1, c2, s1, s2
821 PARAMETER (m = 3) ! number of search directions
822 DIMENSION beta(m), c1(m), c2(m,m), s1(m), s2(m,m)
823
824 COMMON /space3/ ox, z, cgrad, sgrad, xi, eta
825 DIMENSION ox(MaxPts), z(MaxPts)
826 DIMENSION cgrad(MaxBin), sgrad(MaxBin)
827 DIMENSION xi(MaxBin,3), eta(MaxPts,3)
828
829 PARAMETER (TstLim = 0.05) ! for convergence
830 DATA one, zero /1.0, 0.0/ ! compiler-independence!
831
832 WRITE (*,*) ' MaxEnt routine beginning ...'
833
834 chizer = FLOAT(npt)
835 chtarg = chizer
836 blank = flat
837 expl = EXP(one)
838
839 IF (blank .EQ. zero) THEN
840 DO i = 1, n
841 blank = blank + base(i)
842 f(i) = base(i) ! given initial distribution
843 END DO
844 blank = blank / FLOAT(n)
845 WRITE (*,*) ' Average of BASE = ', blank
846 ELSE
847 WRITE (*,*) ' Setting BASE constant at ', blank
848 DO i = 1, n
849 base(i) = blank
850 f(i) = blank ! featureless initial distribution
851 END DO
852 ENDIF
853
854 iter = 0
855 6 iter = iter + 1 ! The iteration loop begins here!
856 CALL opus (n, npt, f, ox) ! calc. the model intensity from "f"
857 chisq = zero
858 DO j = 1, npt
859 a = (ox(j) - datum(j)) / sigma(j)
860 chisq = chisq + a**2
861 ox(j) = 2. * a / sigma(j)
862 END DO
863 CALL tropus(n,npt,ox,cgrad) ! cGradient = Grid * ox
864 test = zero ! mismatch between entropy and ChiSquared gradients
865 snorm = zero ! entropy term
866 cnorm = zero ! ChiSqr term
867 tnorm = zero ! norm for the gradient term TEST
868 fSum = zero ! find the sum of the f-vector
869 DO i = 1, n
870 fSum = fSum + f(i)
871 sgrad(i) = -LOG(f(i)/base(i)) / (base(i)*expl)
872 snorm = snorm + f(i) * sgrad(i)**2
873 cnorm = cnorm + f(i) * cgrad(i)**2
874 tnorm = tnorm + f(i) * sgrad(i) * cgrad(i)

```

```

875 END DO
876 snorm = SQRT(snorm)
877 cnorm = SQRT(cnorm)
878 a = one
879 b = one / cnorm
880 IF (iter .GT. 1) THEN
881     test = SQRT(0.5*(one-tnorm/(snorm*cnorm)))
882     a = 0.5 / (snorm * test)
883     b = 0.5 * b / test
884 ENDIF
885 DO i = 1, n
886     xi(i,1) = f(i) * cgrad(i) / cnorm
887     xi(i,2) = f(i) * (a * sgrad(i) - b * cgrad(i))
888 END DO
889 CALL opus (n,npt,xi(1,1),eta(1,1))
890 CALL opus (n,npt,xi(1,2),eta(1,2))
891 DO j = 1, npt
892     ox(j) = eta(j,2) / (sigma(j)**2)
893 END DO
894 CALL tropus (n,npt,ox,xi(1,3))
895 a = zero
896 DO i = 1, n
897     b = f(i) * xi(i,3)
898     a = a + b * xi(i,3)
899     xi(i,3) = b
900 END DO
901 a = one / SQRT(a)
902 DO i = 1, n
903     xi(i,3) = a * xi(i,3)
904 END DO
905 CALL opus (n,npt,xi(1,3),eta(1,3))
906 DO k = 1, m
907     s1(k) = zero
908     c1(k) = zero
909     DO i = 1, n
910         s1(k) = s1(k) + xi(i,k) * sgrad(i)
911         c1(k) = c1(k) + xi(i,k) * cgrad(i)
912     END DO
913     c1(k) = c1(k) / chisq
914 END DO
915 DO k = 1, m
916     DO l = 1, k
917         s2(k,l) = zero
918         c2(k,l) = zero
919         DO i = 1, n
920             s2(k,l) = s2(k,l) - xi(i,k) * xi(i,l) / f(i)
921         END DO
922         DO j = 1, npt
923             c2(k,l) = c2(k,l) + eta(j,k) * eta(j,l) / (sigma(j)**2)
924         END DO
925         s2(k,l) = s2(k,l) / blank
926         c2(k,l) = 2. * c2(k,l) / chisq
927     END DO
928 END DO
929 c2(1,2) = c2(2,1)
930 c2(1,3) = c2(3,1)
931 c2(2,3) = c2(3,2)
932 s2(1,2) = s2(2,1)

```

```

933     s2(1,3) = s2(3,1)
934     s2(2,3) = s2(3,2)
935     beta(1) = -0.5 * c1(1) / c2(1,1)
936     beta(2) = zero
937     beta(3) = zero
938     IF (iter .GT. 1) CALL Move(m)
939
940 C Modify the current distribution (f-vector)
941     fSum = zero      ! find the sum of the f-vector
942     fChange = zero   ! and how much did it change?
943     DO i = 1, n
944         df = beta(1)*xi(i,1)+beta(2)*xi(i,2)+beta(3)*xi(i,3)
945         IF (df .LT. -f(i)) df = 0.001 * base(i) - f(i)      ! a patch
946         f(i) = f(i) + df      ! adjust the f-vector
947         fSum = fSum + f(i)
948         fChange = fChange + df
949     END DO
950
951     s = zero
952     DO i = 1, n
953         temp = f(i) / fSum      ! fraction of f(i) in this bin
954         s = s - temp * LOG (temp) ! from Skilling and Bryan, eq. 1
955     END DO
956
957     CALL opus (n, nPt, f, z)      ! model the data-space from f(*)
958     ChiSq = zero                  ! get the new ChiSquared
959     DO j = 1, nPt
960         z(j) = (datum(j) - z(j)) / sigma(j)      ! the residuals
961         ChiSq = ChiSq + z(j)**2      ! report this ChiSq, not the one above
962     END DO
963
964 300 IF ( MOD(iter, 5) .EQ. 0 ) THEN
965     WRITE (*,*)
966     WRITE (*,*) ' Residuals'
967     CALL ResPlt (npt, z)
968
969     WRITE (*,*)
970     WRITE (*,*) ' Distribution'
971     CALL BasPlt (n, f, base)
972 END IF
973
974 WRITE (*,*) ' #', iter, ' of ', itermax, ', n = ', npt
975 WRITE (*,200) test, s
976 WRITE (*,201) 'target', SQRT(chtarg/npt), 'now', SQRT(chisq/npt)
977 WRITE (*,202) 'sum', fSum, ' % change', 100.*fChange/fSum
978 200 FORMAT (' test = ', F9.5, ', Entropy = ', F12.7)
979 201 FORMAT (' SQRT((Chi^2)/n):', A8, ' = ', F12.8, A10, ' = ', F12.8)
980 202 FORMAT (' f-vector:', A8, ' = ', F12.8, A10, ' = ', F12.8)
981
982 C See if we have finished our task.
983 IF (ABS(chisq/chizer-one) .LT. 0.01) THEN ! hardest test first
984     IF (test .LT. TstLim) THEN          ! same solution gradient?
985 C         We've solved it but now must check for a bizarre condition.
986 C         Calling routine says we failed if "iter = iterMax".
987 C         Let's increment iterMax so (maybe) this doesn't happen.
988         IF (iter .EQ. iterMax) iterMax = iterMax + 1
989         RETURN
990     END IF

```

```

991     END IF
992     IF (iter .LT. iterMax) GO TO 6
993
994 C Ask for more time to finish the job.
995     WRITE (*,*)
996     WRITE (*,*) ' Maximum iterations have been reached.'
997 2001  WRITE (*,*) ' How many more iterations? <none>'
998     READ (*,'(I4)') more
999     IF (more .LT. 0) GO TO 2001
1000    IF (more .EQ. 0) RETURN
1001    iterMax = iterMax + more
1002    GO TO 6
1003    END
1004
1005
1006 SUBROUTINE Move(m)
1007 IMPLICIT REAL*8 (A-H,O-Z)
1008 IMPLICIT INTEGER*4 (I-N)
1009 PARAMETER ( MxLoop = 500 ) ! for no solution
1010 PARAMETER ( Passes = 1.e-3 ) ! convergence test
1011 COMMON /space5/ chisq, chtarg, chizer, fSum, blank
1012 COMMON /space2/ beta, c1, c2, s1, s2
1013 DIMENSION beta(3), c1(3), c2(3,3), s1(3), s2(3,3)
1014 DATA one, zero /1.0, 0.0/ ! compiler-independence!
1015 a1 = zero ! lower bracket "a"
1016 a2 = one ! upper bracket of "a"
1017 cmin = ChiNow (a1, m)
1018 IF (cmin*chisq .GT. chizer) ctarg = 0.5*(one + cmin)
1019 IF (cmin*chisq .LE. chizer) ctarg = chizer/chisq
1020 f1 = cmin - ctarg
1021 f2 = ChiNow (a2,m) - ctarg
1022 DO loop = 1, MxLoop
1023     anew = 0.5 * (a1+a2) ! choose a new "a"
1024     fx = ChiNow (anew,m) - ctarg
1025     IF (f1*fx .GT. zero) a1 = anew
1026     IF (f1*fx .GT. zero) f1 = fx
1027     IF (f2*fx .GT. zero) a2 = anew
1028     IF (f2*fx .GT. zero) f2 = fx
1029     IF (abs(fx) .LT. Passes) GO TO 2
1030 END DO
1031
1032 C If the preceding loop finishes, then we do not seem to be converging.
1033 C Stop gracefully because not every computer uses control-C (etc.)
1034 C as an exit procedure.
1035 WRITE (*,*) ' Loop counter = ', MxLoop
1036 PAUSE ' No convergence in alpha chop (MOVE). Press return ...'
1037 STOP ' Program cannot continue.'
1038
1039 2 w = Dist (m)
1040 IF (w .GT. 0.1*fSum/blank) THEN
1041     DO k = 1, m
1042         beta(k) = beta(k) * SQRT(0.1 * fSum/(blank * w))
1043     END DO
1044 END IF
1045 chtarg = ctarg * chisq
1046 RETURN
1047 END
1048

```

```

1049
1050 REAL*8 FUNCTION Dist (m)
1051 IMPLICIT REAL*8 (A-H,O-Z)
1052 IMPLICIT INTEGER*4 (I-N)
1053 COMMON /space5/ chisq, chtarg, chizer, fSum, blank
1054 COMMON /space2/ beta, c1, c2, s1, s2
1055 DIMENSION beta(3), c1(3), c2(3,3), s1(3), s2(3,3)
1056 DATA one, zero /1.0, 0.0/ ! compiler-independence!
1057 w = zero
1058 DO k = 1, m
1059     z = zero
1060     DO l = 1, m
1061         z = z - s2(k,l) * beta(l)
1062     END DO
1063     w = w + beta(k) * z
1064 END DO
1065 Dist = w
1066 RETURN
1067 END
1068
1069
1070 REAL*8 FUNCTION ChiNow(ax,m)
1071 IMPLICIT REAL*8 (A-H,O-Z)
1072 IMPLICIT INTEGER*4 (I-N)
1073 COMMON /space5/ chisq, chtarg, chizer, fSum, blank
1074 COMMON /space2/ beta, c1, c2, s1, s2
1075 DIMENSION beta(3), c1(3), c2(3,3), s1(3), s2(3,3)
1076 DIMENSION a(3,3), b(3)
1077 DATA one, zero /1.0, 0.0/ ! compiler-independence!
1078 bx = one - ax
1079 DO k = 1, m
1080     DO l = 1, m
1081         a(k,l) = bx * c2(k,l) - ax * s2(k,l)
1082     END DO
1083     b(k) = -(bx * c1(k) - ax * s1(k))
1084 END DO
1085 CALL ChoSol(a,b,m,beta)
1086 w = zero
1087 DO k = 1, m
1088     z = zero
1089     DO l = 1, m
1090         z = z + c2(k,l) * beta(l)
1091     END DO
1092     w = w + beta(k) * (c1(k) + 0.5 * z)
1093 END DO
1094 ChiNow = one + w
1095 RETURN
1096 END
1097
1098
1099 SUBROUTINE ChoSol(a, b, n, beta)
1100 IMPLICIT REAL*8 (A-H,O-Z)
1101 IMPLICIT INTEGER*4 (I-N)
1102 DIMENSION fl(3,3), a(3,3), bl(3), b(3), beta(3)
1103 DATA one, zero /1.0, 0.0/ ! compiler-independence!
1104 IF (a(1,1) .LE. zero) THEN
1105     WRITE (*,*) ' Fatal error in CHOSOL: a(1,1) = ', a(1,1)
1106     PAUSE ' Press <RETURN> to end program ...'

```

```

1107     STOP ' Program cannot continue.'
1108 END IF
1109 fl(1,1) = SQRT(a(1,1))
1110 DO   i = 2, n
1111     fl(i,1) = a(i,1) / fl(1,1)
1112     DO   j = 2, i
1113         z = zero
1114         DO   k = 1, j-1
1115             z = z + fl(i,k) * fl(j,k)
1116         END DO
1117         z = a(i,j) - z
1118         IF (j .EQ. i) fl(i,j) = SQRT(z)
1119         IF (j .NE. i) fl(i,j) = z / fl(j,j)
1120     END DO
1121 END DO
1122 bl(1) = b(1) / fl(1,1)
1123 DO   i=2, n
1124     z = zero
1125     DO   k = 1, i-1
1126         z = z + fl(i,k) * bl(k)
1127     END DO
1128     bl(i) = (b(i) - z) / fl(i,i)
1129 END DO
1130 beta(n) = bl(n) / fl(n,n)
1131 DO   i1 = 1, n-1
1132     i = n - i1
1133     z = zero
1134     DO   k = i+1, n
1135         z = z + fl(k,i) * beta(k)
1136     END DO
1137     beta(i) = (bl(i) - z) / fl(i,i)
1138 END DO
1139 RETURN
1140 END
1141
1142
1143 SUBROUTINE ResPlt (n, x)
1144 C Draw a plot of the standardized residuals on the screen.
1145 C Mark the rows of + and - one standard deviation.
1146 IMPLICIT REAL*8 (A-H,O-Z)
1147 IMPLICIT INTEGER*4 (I-N)
1148 DIMENSION x(1)
1149 CHARACTER*1 Blank, Symbol, hBordr, vBordr, resSym
1150 PARAMETER (Blank = ' ', Symbol = 'O', resSym = '=')
1151 PARAMETER (hBordr = '-', vBordr = '|')
1152
1153 COMMON /space4/ screen, MaxCol, MaxRow, MxC2, MxR2
1154 CHARACTER*1 screen(100, 150)
1155
1156     IF (n .LT. 2) RETURN      ! not enough data
1157
1158 C Find out how many points to pack per column and how many columns
1159     nPack = 1 + INT(FLOAT (n) / MaxCol - 1./n)
1160     nCol = INT((n - 1./n)/nPack + 1)
1161
1162 C prepare the "screen" for drawing
1163     DO   j = 1, nCol + 2
1164         DO   i = 1, MxR2

```

```

1165     screen(i,j) = Blank
1166     END DO
1167 END DO
1168 DO   i = 2, nCol + 1
1169     screen(MxR2,i) = hBordr
1170     screen(1,i) = hBordr
1171 END DO
1172 DO   i = 2, MaxRow + 1
1173     screen(i,nCol+2) = vBordr
1174     screen(i,1) = vBordr
1175 END DO
1176
1177 C get the data limits
1178     xMax = 1.
1179     xMin = -1.
1180     DO i = 1, n
1181     IF (x(i) .GT. xMax) xMax = x(i)
1182     IF (x(i) .LT. xMin) xMin = x(i)
1183 END DO
1184     RowDel = (MaxRow - 1) / (xMax - xMin)
1185
1186 C show the standard deviation bars
1187     mPlus = 1 + INT((1 - xMin)*RowDel + 1)
1188     mMinus = 1 + INT((-1 - xMin)*RowDel + 1)
1189     DO i = 2, nCol + 1
1190     screen(mMinus,i) = resSym
1191     screen(mPlus,i) = resSym
1192 END DO
1193
1194 C draw the data (overdrawing the residuals bars if necessary)
1195     DO i = 1, n
1196     mCol = 1 + INT((i - 1./n)/nPack + 1)      ! addressing function
1197     mRow = 1 + INT((x(i) - xMin)*RowDel + 1) ! +1 for the plot frame
1198     screen(mRow, mCol) = Symbol
1199 END DO
1200
1201 C convey the "screen" to the default output
1202 WRITE (*,*) nPack, ' point(s) per column'
1203 WRITE (*,*) 1./RowDel, ' standard deviations per row'
1204 DO i = MxR2, 1, -1
1205     WRITE (*,*) (screen(i,j), j = 1, nCol + 2)
1206 END DO
1207
1208 RETURN
1209 END
1210
1211
1212 SUBROUTINE BasPlt (n, x, basis)
1213 C Draw a plot of some data with reference to a basis line on the plot.
1214 C The basis is that line below which the data is not meaningful.
1215 IMPLICIT REAL*8 (A-H,O-Z)
1216 IMPLICIT INTEGER*4 (I-N)
1217 DIMENSION x(1), basis(1)
1218 CHARACTER*1 Blank, Symbol, hBordr, vBordr, BasSym
1219 PARAMETER (Blank = ' ', Symbol = 'O', BasSym = '=')
1220 PARAMETER (hBordr = '-', vBordr = '|')
1221
1222 COMMON /space4/ screen, MaxCol, MaxRow, MxC2, MxR2

```

```

1223 CHARACTER*1 screen(100, 150)
1224
1225     IF (n .LT. 2) RETURN      ! not enough data
1226
1227 C Find out how many points to pack per column and how many columns
1228     nPack = 1 + INT(FLOAT (n) / MaxCol - 1./n)
1229     nCol = INT((n - 1./n)/nPack + 1)
1230
1231 C prepare the "screen" for drawing
1232     DO j = 1, nCol + 2
1233         DO i = 1, MxR2
1234             screen(i,j) = Blank
1235         END DO
1236     END DO
1237     DO i = 2, nCol + 1
1238         screen(MxR2,i) = hBordr
1239         screen(1,i) = hBordr
1240     END DO
1241     DO i = 2, MaxRow + 1
1242         screen(i,nCol+2) = vBordr
1243         screen(i,1) = vBordr
1244     END DO
1245
1246 C get the data limits
1247     xMax = x(1)
1248     xMin = xMax
1249     DO i = 1, n
1250         IF (x(i) .GT. xMax) xMax = x(i)
1251         IF (x(i) .LT. xMin) xMin = x(i)
1252         IF (basis(i) .GT. xMax) xMax = basis(i)
1253         IF (basis(i) .LT. xMin) xMin = basis(i)
1254     END DO
1255     RowDel = (MaxRow - 1) / (xMax - xMin)
1256
1257
1258 C draw the data (overdrawing the basis bars if necessary)
1259     DO i = 1, n
1260         mCol = 1 + INT((i - 1./n)/nPack + 1)      ! addressing function
1261         mRow = 1 + INT((basis(i) - xMin)*RowDel + 1) ! basis
1262         screen(mRow, mCol) = basSym
1263         mRow = 1 + INT((x(i) - xMin)*RowDel + 1) ! data
1264         screen(mRow, mCol) = Symbol
1265     END DO
1266
1267 C convey the "screen" to the default output
1268     WRITE (*,*) nPack, ' point(s) per column'
1269     WRITE (*,*) 1./RowDel, ' units per row'
1270     DO i = MxR2, 1, -1
1271         WRITE (*,*) (screen(i,j), j = 1, nCol + 2)
1272     END DO
1273
1274     RETURN
1275     END
1276
1277
1278     SUBROUTINE Plot (n,x,y)
1279 C Make a scatter plot on the default display device (UNIT=*).
1280 C MaxRow and MaxCol correspond to the display dimensions.

```

```

1281 IMPLICIT REAL*8 (A-H,O-Z)
1282 IMPLICIT INTEGER*4 (I-N)
1283 DIMENSION x(1), y(1)
1284 CHARACTER*1 Blank, Symbol, hBordr, vBordr
1285 PARAMETER (Blank = ' ', Symbol = 'O')
1286 PARAMETER (hBordr = '-', vBordr = '|')
1287
1288 COMMON /space4/ screen, MaxCol, MaxRow, MxC2, MxR2
1289 CHARACTER*1 screen(100, 150)
1290
1291     IF (n .LT. 2) RETURN      ! not enough data
1292
1293 C  prepare the "screen" for drawing
1294     DO   j = 1, MxC2
1295         DO   i = 1, MxR2
1296             screen(i,j) = Blank
1297         END DO
1298     END DO
1299     DO   i = 2, MaxCol+1
1300         screen(MxR2,i) = hBordr
1301         screen(1,i) = hBordr
1302     END DO
1303     DO   i = 2, MaxRow+1
1304         screen(i,MxC2) = vBordr
1305         screen(i,1) = vBordr
1306     END DO
1307
1308 C  get the data limits
1309     xMin = x(1)
1310     xMax = x(1)
1311     yMin = y(1)
1312     yMax = y(1)
1313     DO   i = 2, n
1314         IF (x(i).GT.xMax) xMax=x(i)
1315         IF (x(i).LT.xMin) xMin=x(i)
1316         IF (y(i).GT.yMax) yMax=y(i)
1317         IF (y(i).LT.yMin) yMin=y(i)
1318     END DO
1319     ColDel = (MaxCol - 1) / (xMax - xMin)
1320     RowDel = (MaxRow - 1) / (yMax - yMin)
1321
1322 C  data scaling functions are offset by +1 for plot frame
1323     DO   i = 1, n
1324         mCol = 1 + INT((x(i) - xMin)*ColDel + 1)
1325         mRow = 1 + INT((y(i) - yMin)*RowDel + 1)
1326         screen(mRow, mCol) = Symbol
1327     END DO
1328
1329 C  convey the "screen" to the default output
1330     WRITE (*,*) 1./ColDel, ' units per column'
1331     WRITE (*,*) 1./RowDel, ' units per row'
1332     DO   i = MaxRow + 2, 1, -1
1333         WRITE (*,*) (screen(i,j), j = 1, MaxCol + 2)
1334     END DO
1335     RETURN
1336     END

```

1.4.10 Last Ditch Help

Any user who has, without success, tried all of the suggestions provided in the section titled *OBSERVATIONS, HINTS, SUGGESTIONS* for correcting a failure of the program should feel free to contact the authors listed here at any time for further advice and suggestions.

1.4.11 References

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