Using Spectral Line Profiles as a Diagnostic of the Plasma Electron Density

by

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ABSTRACT

A description of a simple interactive fitting procedure is given which uses line profiles calculated for highly stripped ions, i.e., hydrogenic, helium-like and lithium-like species. Information on the calculation of these profiles is provided. The experimental data is read from disk, so any appropriately formatted data can be referenced.

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I. Introduction

The use of spectral-line profiles as a diagnostic tool for plasma electron density has been well-documented since the hydrogen n = 2 to n = 4 transition, $H\beta$, was first used as a measure of stellar atmospheric electron density. In our case we are interested in more than the hydrogen-line profiles. We attempt to use certain hydrogenic, helium-like and lithium-like profiles that are emitted by ions in various plasma sources. Our attention is focussed on the line shape as a function of plasma electron density, n_e, since if the line emission is optically thin, the fit between the emitted profile and the theoretical curve should yield a measure of the plasma density. Unfortunately, in practice, there are many assumptions which must be proved valid before we can give any clear indication of the accuracy of the n_e determination. These assumptions are:

A) The line shape is not dominated by instrument function, i.e., the instrument width << intrinsic line width.

B) The temperature of the plasma can be ascertained to a degree of accuracy to ensure that:

1) The temperature variation of the collisional broadening does not modify the profile, so the same fit is obtained for a wide range of n_e within the temperature range, and

2) The thermal Doppler effect should be small compared to the intrinsic width of the line profile. If this is not true, the line is a temperature diagnostic.

C) The line is optically thin, so the width, and shape, are functions of local plasma conditions, not the radiation transfer. (For methods where optically thick lines can be used as a diagnostic, see Appendices).

D) The quality of the data and theory justify the degree of accuracy derivable in the fitting procedure. (For a method of analyzing noisy data see Appendix 1).

If these constraints have been met, the line shape with its various features, e.g., slope, width and adjacent components can be an accurate diagnostic. However, in reality, only in experiments specifically designed to do line-shape studies are all these requirements met. Therefore, the nature of this fitting procedure is to facilitate line-shape diagnostics in both the ideal and normal cases.

II. General Comments on the Program

The program, called FIT, and the controlee RUNFIT can be found on .575314:RWLEE. It is an FTN program and runs compatibly with the line profile programs described in document UCID #18876. The basic requirements are to have an experimental data set with two header lines and spectral data, one energy and intensity per line (energy in EV), and some theoretically calculated profiles (the calculation of which are described in UCID-18876) both on disk. One starts the program, inputs the data interactively, initiates the fitting by lining up the two sets of data, and proceeds to fit the profiles by monitoring TMDS frames. This procedure can be repeated for new data, either experimental and/or theoretical. The output is a picture file of the fits, which can be viewed using UXTV, and a print file TOUT, which contains hardcopy of all the fitting performed in a run.

III. Running the Program

Note that FTN produces prompts, i.e., a "?", when it wants data; and further, it accepts free format input either space, or comma delimited.

However, if n items are asked for, n entries must be made, except when carriage return (denoted CR below), which implies a default is acceptable for the entire input string.

The program is most easily discussed in three sections:

A) Input

1) Experimental Data Set (No Default)

When the program starts, the first input is the experimental data set name, which must be no greater than 10 characters. This must be entered; there is no default.

2) Instrumental Line Shape (Default Allowed)

The next input is the instrument half-half width, in EV, and the type of instrument function 1 = Lorentzian, 0 = Gaussian. The default, i.e., a CR response, yields a Lorenztian with a half-half width of .025 EV.

3) Profile Information (No Defaults)

The request for input profile information requires three numbers:

a) Input Profile Number:

This is the number denoting which transition of a particular element is required. See Table I for the full list of numbers.

b) Element:

This is request for the ion species type;
1 = hydrogenic, 2 = helium-like, 3 = lithium-like.

Note: the number must correlate correctly with the theoretical data set (see II.A.4 below), or the input data will be read incorrectly.

c) Energy:

This is the fine center energy of the transition of interest if you know that there is an offset in the data. First time through put 0.0, thereafter having seen data, an offset can be input (see II.B. below). This can speed up program execution.

4) Theoretical Data Set (No Default)

This is the name of the disk file that contains the data to be fit. It must be less than, or equal to, 10 characters.

B) Initialization:

In this part of the code, a picture of both the experimental and theoretical profiles are shown. The object is to verify that the profiles are in the correct position without having to fit them, and provides a quick look at the data. The method is to show the experimental data for five times the total theoretical energy range, or less if it does not exist. The intensity normalization is done to peak heights, so a view of both profiles should be obtained. The program then writes the offset (i.e. the data shift which is applied to the theoretical energy scale to obtain a best first-pass correspondence between the two profiles) and requests an input offset. The valid responses are:

1) Number (+,0,-) indicates another pass is to be made to shift the whole theoretical data set. A + number moves the theory to higher energy by + number eV. The next response will be a request for a new offset.

2) CR indicates that the data are lined up close enough to fit. The next response will be for fitting information (see III. C below).

3) -9999. indicates a restart with a new theoretical data set. This can occur when the present data set is obviously not going to fit (e.g. it is much too wide when optically thin). The next response will be a request for profile name (see II. A. 4).

Note: The offset can be used in subsequent fits in the energy input (see II. A. 3) if a common bias is found.

C) Fitting

Once the offset has been determined, the energy of the theoretical data is considered fixed. Now the program requires information on the detailed fitting of the profiles. The requests in the order of their occurrence and the appropriate responses are listed below:

1) Request for ℓ and n/cc

The information requested here is the geometrical path length in cm and the ground state ion number density of the transition in number/cc. This is used in a simple slab-geometry optical depth model. $I_{out} = B\ (1-e^{-\tau})$ where B is the black body source function at the plasma temperature and $\tau = \phi k n$ with ϕ the line profile.

a) CR indicates the values shown are acceptable.

b) Input ℓ and n/cc.

Note: Do not allow ℓ = 0, n/cc = 0 to be used. The program will fail.

2) Request for Shift

This is attempting to "fine tune" the relative positions of the two profiles. Note carefully that these shifts do not permanently shift the data (unlike OFFSET-see II. B.). The responses are:

a) +,0,-numbers moves the experimental profile such that + numbers move experimental data to lower energy.

b) 1N indicates present shift will be used.

c) -9999. indicates desire to stop program.

d) 9999. indicates desire to input new number for theoretical data the next response will be for profile information (See section II. A. 3.).

3) Request for Information on Type of Fitting

There are four possibilities with the present program:

a. Scaling to a given data point,

b. Area normalization,

c. No modifications, i.e., just plotting and,

d. A least squares fit.

A) + Number indicates that the n^{th} experimental point, (arrived at by starting from the first experimental point which overlaps the theory at low energy) will be used to scale the profiles. On the plot an "A" will appear at this point.

B) 0 indicates that the curves will be area normalized by taking only the points of overlap.

C) - Number indicates that nothing will be done to the data before plotting. This is only useful if you believe you have an LTE radiator of fixed and n/cc and have absolute experimental data since $I_{OUT}^{THEORY} = B(1-e^{-T})$.

D) CR indicates that a least squares fit is desired. In this case the program requests information concerning which overlapped points are to be used. The program returns the first and last point initially. The valid responses are:

i) N, N^1: (where N, N^1 are two numbers within the range specified) indicates the fit occurs between points N and N^1.

ii) CR: indicates the points already printed are satisfactory. In this case, the plot will have two "X"s to denote the boundaries of the fit.

4) Request for Next Step

The program prints out the temperature, density & and n/cc and requests information on the next step. The responses are:

a) "1": indicates stop program.

b) "2": indicates another fit with the same data is desired; the next request will be for shift (see III. C. 2.).

c) "3": indicates a desire to change optical depth; the next request will be for & and n/cc (see III. C. 1.).

d) "4": indicates a desire to change theoretical data; the next request will be for profile information (see III.A.3.).

e) "5": indicates a desire to change experimental data set; the next request will be for experimental profile name (see III.A.1.).

f) CR: indicates the same as input "2".

IV. Outputs

The outputs of the program are in two forms, TUMS graphs (see Fig. 1) and printout. In addition, at the end of a particular run, the graphics file is present as a UVBU file which can be processed by using UXTV.

A) Pictures

There are two types of pictures, one for the initialization sequence (see III.B.) and one for the fitting sequence (see III.C.).

1) Common Plot Features

The common features of the two plots are the labelling and the axes. First, in the upper left hand corner is a two-line information block of the profiles. Line one contains the ion type, atomic number and the transition number. Line two is temperature, density and $n\ell/cc$ product for the fit. Above the plot is one line containing information to assist in estimating the quality of fit, the shift, the normalized sum of the squares for deviation between the profiles, the experimental half width and the theoretical half width.

Further, the abscissa is in eV and the ordinate is in relative intensity units.

2) Differences in Two Plots

The differences in the two profiles are the following:

a) The initialization plot has the experimental data points marked by "*" and connected by solid-line segments. The theoretical data is denoted by a dotted line.

b) The fitting plots have the experimental points labeled with an "*" and the theoretical curve is a continuous line. In addition, if the scaling or least squares fitting options are chosen one or two "A"s will appear to denote the points of interest (see III.C.3.).

B) Hardcopy

The file TOUT is created for each run. It is rewound and then written over, so it must be dealt with before rerunning to be saved. The information on the file contains the data set names, the temperature and density of the theoretical data, the type of fit and its parameters. That is, the generalized fit is given an input profile I(w) and energies w. The final fitted data is

$$I_{FIT} = A * I (W-\Delta) + B$$

where

A = scale factor
B = continuum level
Δ = shift.

Then the experimental data, original theory, the new theoretical data and the energy are printed. Finally, the half widths are printed.

Appendix 1: Procedure for Obtaining n_e from the Wings of a Line.

In certain cases, the line cores are not reliable either because the opacity and n_e density are not known or because the line core has saturated the detection system. (See Appendix 2 for cases where the signal-to-noise ratio is low, but a series of lines are present.)

Smith and Peacock (J. Phys B, 11, 2749, (1979)) have pointed out that if one can ascertain a point in the line wing, which is known absolutely, then the region slightly beyond the half width can be fit and an electron density determined. Essentially, the method would be to pick a point in the wing by using the scaling option for a series of different theoretical profiles. This requires a reasonable knowledge of the plasma Z, but this is not crucial. (See R. W. Lee and A. J. Freeman, JQSRT, 24, 43 (1980) for the sensitivity of the microfield, which is at question here, to the perturber charge. The fact that one can use the full calculations to generate the profile into the near line wing is a useful extension of the technique. The fits should be accurate to 20% if one can obtain an absolute intensity.

Appendix 2: Procedures for Obtaining Plasma Parameter From Series of Lines

In the case where a series of low-signal-to-noise ratio is present, some optically thick and at least one optically thin, the program can be used to find not only the electron density but also the ground state number density, n_1. The basic concept is to use equal area normalization and ascertain the best fits consistently for all lines.

Although other fitting procedures such as a least squares fit were tested, it was felt that area normalization maintained the most objective fitting procedure. To characterize the quality of the fit, a normalized sum of the squares parameter S was used. This S is defined by:

$$S = \Sigma(Y_{exp} - Y_{th})^2 \; \Delta Y_{th}^{-2}$$

and is printed out on the top of each plot. Here y_{exp} and t_{th} are the experimental and theoretical points at the same wavelength, and the sum is over all of the digitized experimental points. In general, a fit with Q = .01 is good, whereas a fit with Q = 0.1 is poor.

The two major variables in determining the width of the observed emission line are n_e and n_1 for a given ℓ. The gross width of any line is not a unique function of n_e and n_1. The details of a line shape, e.g. the height of shoulders, may be a unique function of n_e and n_1, but it is only the coarse features that are observable. If the theory is compared with a given experimental profile, then for small optical depth the line width will be a function of n_e only, and if the line of best fit is plotted on graph of n_e versus $n_1\ell$ as in Fig. 2, it will be a horizontal line. As the line becomes optically thick, the same total theoretical width can be obtained with a smaller n_e. Thus, the line of best fit curves downwards as in Fig. 2. Ideally, a line of best fit could be obtained for several transitions, and they would intersect at one point in the n_e, $n_1\ell$ plot, characterizing n_e and n_1 in the slab.

In fact, the line of fit is an area, determined by the constaint on Q which can be taken as $Q < 2\,Q_{min}$ where Q_{min} is the quality of the best fit. Thus, instead of a point in n_e, $n_1 \ell$ space, an area should be defined by the common overlapping area of several transitions.

The maximum number density of ionization the stage of interest can also be represented on the n_e n_1 plot. If, for example, the plasma is of one element of atomic density n_a, and average charge Z

$$n_H < 0.5\, n_a = \frac{0.5}{Z}\, n_e$$

thus describing an allowed region in the n_e, n_1 parameter space. The end result is fit with a set of error bounds indicating the quality of the data and the sensitivity of the theory.

The outputs of the program, both graphical and hardcopy, can be used as aids in fitting line profiles with this method.

Appendix 3: Running Job From Source

To obtain the program FIT from storage and run it, one needs to get it from .575314.RWLEE. Then, since it is an FTN program that uses graphic, the graphic file FTNTV80 must be used. To get this use

```
EXE LASLFTN FTNTV80 DR. / T V
```

To run the program, use the following:

```
FTN (I=FIT,L=O,CNAME=RUNFIT,SYM=S, GLIB=FTNTV80,GO) / T V
```

This will create the controllee RUNFIT and start execution of the job. The compilation listing is on "O".

Appendix 4: Obtaining Hardcopy of Plots

In general, the plot files will be UX files with names like UALFTNUD8U. The files can be processed in any manner, however, the entire UX file processing system is not well-documented. Here are two simple choices:

1) UXTV will show the pictures again.

2) UXRJ will send them to an RJET. The input line here is:

UXRJ 27(RJET #), NARROW, FAMILY., UALFTNUD8U(UD8U File),

NORM, MUUZ. .735 ALL.

The graphs will then fit on one versatec page.

Table 1 - Key to Input

TRANSITION NUMBER	ELEMENT NUMBER
1 = Lyman α	
2 = Lyman β	1 = Hydrogenic
3 = Lyman γ	
4 = Lyman δ	
5 = Balmer α	
6 = Balmer β	
1 = $1s^2\ {}^1S_0 - 1s2p\ {}^1P$	
2 = $1s^2\ {}^1S_0 - 1s3p\ {}^1P$	2 = Helium-like
3 = $1s^2\ {}^1S_0 - 1s4p\ {}^1P$	

NUMBER

1 = $2S-{}^2P$

2 = $2P_{3/2}$ 3S

3 = $2P_{3/2}$-3D

4 = $2P_{1/2}$-3S

5 = $2P_{1/2}$-3D

6 = 2S-4P

7 = $2P_{3/2}$-4S

8 = $2P_{3/2}$-4D

9 = $2P_{1/2}$-4S

10 = $2P_{1/2}$-4D

ELEMENT NUMBER

9 = Lithium-like

SAMPLE TMDS GRAPH

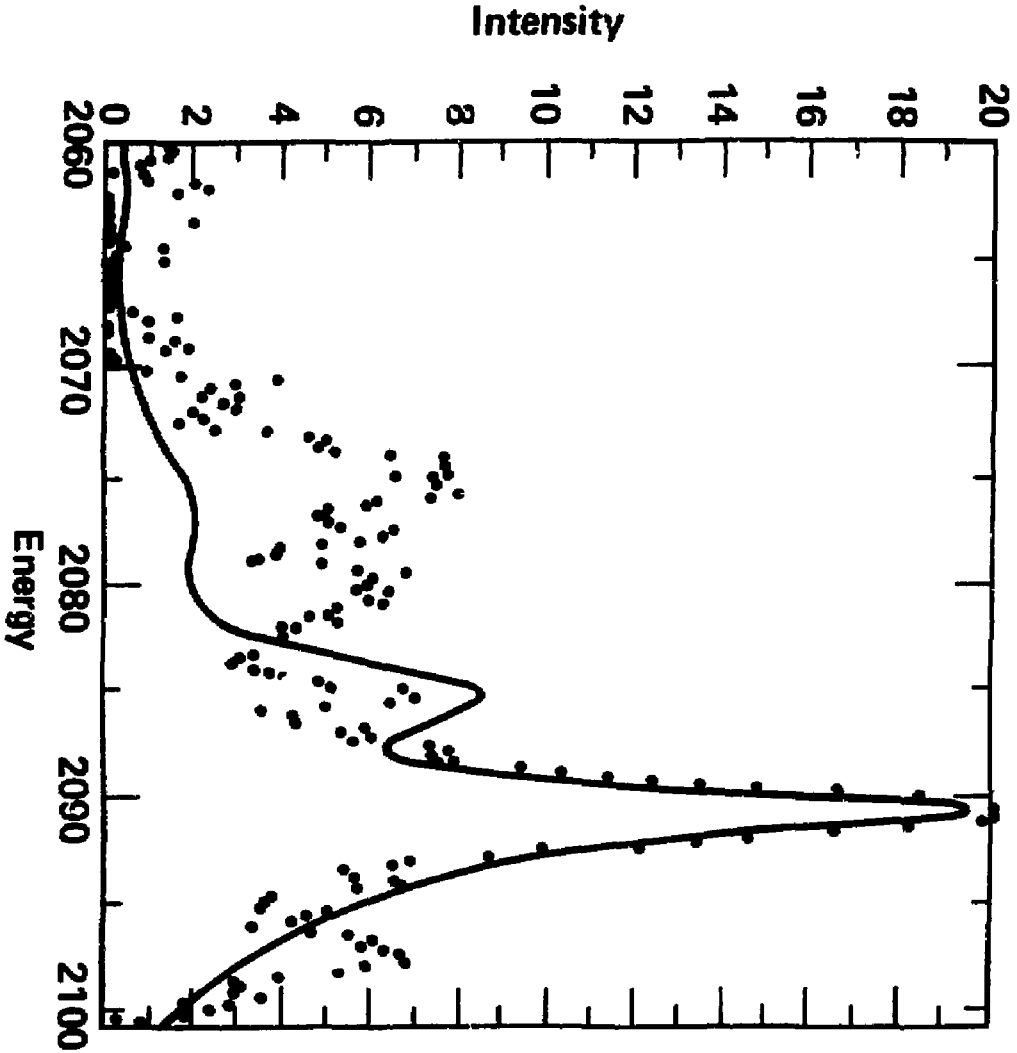

Figure 1

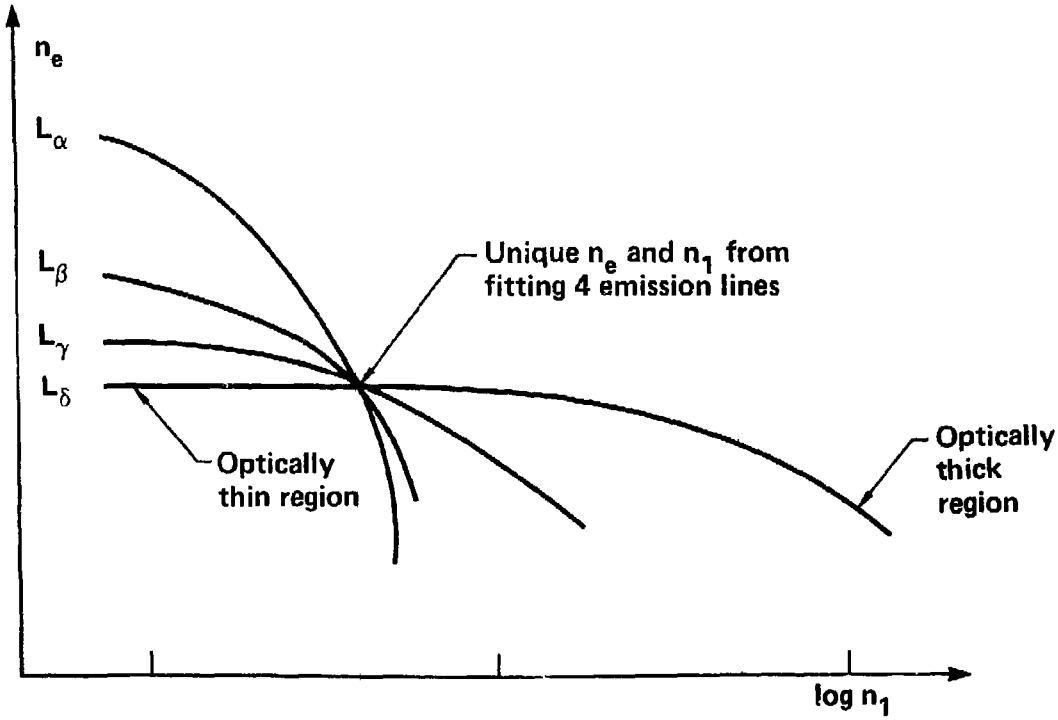

FIGURE 2

IDEAL LINE OF BEST FIT FOR SEVERAL SPECTRAL LINES

SAMPLE EXPERIMENT INPUT FILE

```
538 LINES.  (80A)
  1 SHOT 80090504 ALICE
  2 ENERGY FLUX
  3     2.02650750E+00    1.02992399E+07
  4     2.02671976E+00    9.09302601E+06
  5     2.02693207E+00    8.40534554E+06
  6     2.02714444E+00    8.17915467E+06
  7     2.02735687E+00    8.59371253E+06
  8     2.02756936E+00    8.51728462E+06
  9     2.02778191E+00    7.89837018E+06
 10     2.02799452E+00    8.27759559E+06
 11     2.02820719E+00    8.17497146E+06
 12     2.02841992E+00    7.17470955E+06
 13     2.02863270E+00    5.99938549E+06
 14     2.02884555E+00    5.38121753E+06
 15     2.02905845E+00    4.92032303E+06
 16     2.02927142E+00    4.74637518E+06
 17     2.02948444E+00    4.40869623E+06
 18     2.02969752E+00    4.35621792E+06
 19     2.02991067E+00    4.07177961E+06
 20     2.03012387E+00    3.41025551E+06
...ETC
```

SAMPLE PROGRAM EXECUTION

```
RUNFIT / 10 20
TYPE TMDS MONITOR NUMBER: 732
 INPUT EXPERIMENTAL DATA SET NAME
? EF0504A
 INPUT INSTRUMENT WIDTH IN E' AND TYPE '1=LOR 2=GAUSS'
? .25,1
 INPUT PROFILE NUMBER , ELEMENT AND ENERGY('E')
? 1 1 0
 INPUT NAME OF THEORETICAL DATA SET
? SI11T1P23
 INPUT NEW SHIFT '+ MOVES THEOR, TO HIGHER ENERGY' OR CR IF READY
                    OFFSET =        0.0000
? 3.5
 INPUT NEW SHIFT '+ MOVES THEOR, TO HIGHER ENERGY' OR CR IF READY
                    OFFSET =        3.5000
?
L, AND N-CC NOW =    0.          0.        INPUT VALUES OR CR
? 1E-3,1E20
 INPUT SHIFT '+ MOVES E FT LOWER' IT IS NOW        0.0000
?
 INPUT +N SCALING, 0 AREA, -N NO SCALING, OR LED
? 0
T, NE, L, AND N-CC =     .95E+03   .10E+24   .10E-02   .10E+21
 1=STOP 2=FIT 3=N-CC 4=THEOR, 5=ALL
? 3
L, AND N CC NOW =    1.00E-03  1.00E+20 INPUT VALUES OR CR
? 1E-3,1E21
 INPUT SHIFT '+ MOVES E FT LOWER' IT IS NOW        0.0000
?
 INPUT +N SCALING, 0 AREA, -N NO SCALING, OR LED
? 0
T, NE, L, AND N CC =     .95E+03   .10E+24   .10E-02   .10E+22
 1=STOP 2=FIT 3=N CC 4=THEOR, 5=ALL
? 4
 INPUT PROFILE NUMBER , ELEMENT AND ENERGY('E')
? 1 1 2003
 INPUT NAME OF THEORETICAL DATA SET
? SI11T3P24
 INPUT NEW SHIFT '+ MOVES THEOR, TO HIGHER ENERGY' OR CR IF READY
                    OFFSET =        0.0000
?
L, AND N-CC NOW =    1.00E-03  1.00E+21 INPUT VALUES OR CR
?
 INPUT SHIFT '+ MOVES E-FT LOWER' IT IS NOW        0.0000
? 0
 INPUT +N SCALING, 0 AREA, -N NO SCALING, OR LED
? 0
T, NE, L, AND N-CC =     .10E+04   .32E+25   .10E-02   .10E+22
 1=STOP 2=FIT 3=N-CC 4=THEOR, 5=ALL
? 1
 STOP FTN
RUNFIT      LTSS TIME      5.372 SECONDS
CPU=     2.449        SYS=      .033        I-O=     2.890

 ALL DONE
```