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MIXERG-Generated SESAME-Formatted
Multigroup Opacity Tables**

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March 1987

UWFDM-721

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SESAME-Formatted Multigroup Opacity
Tables**

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UWEOSPAC: A SUBROUTINE PACKAGE FOR ACCESSING MIXERG-GENERATED
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March 1987

UWFD-721

1. Introduction

This document describes UWEOSPAC, a subroutine package for accessing the SESAME-formatted multigroup opacity tables generated by the MIXERG [1] program. It contains problem setup routines for storing multigroup data tables and vectorized search-interpolate routines for table lookup. All of the subroutines in this have come from EOSPAC [2], developed at Los Alamos National Laboratory, and have been modified for use with multigroup data tables. Therefore, acknowledgement is given to Charles W. Cranfill and the others at Los Alamos who developed EOSPAC.

The UWEOSPAC subroutines can be used for interpolating multigroup tables of data which are functions of three independent variables, and where the third independent variable is given as a range of values. For example, the Rosseland opacity is tabulated as a function of mass density, temperature, and photon energy group number. Each energy group is specified by a range, a lower and upper bound, and the ranges are contiguous over all of the groups. Thus the multigroup tables can be thought of as a number of group tables, each tabulating a function of two independent variables.

UWEOSPAC builds upon the vectorized search-interpolate subroutines developed for EOSPAC. UWEOSPAC takes advantage of the fact that for any group table, the indexes of the variables used in the interpolation will be the same as the indexes used in every other group table. Rather than look up these indexes for each group table, the subroutines in UWEOSPAC look up the indexes just once for each pair of independent variables. Then all the group tables are interpolated at once. For the case of twenty group tables, this procedure saves looking up nineteen sets of indexes and improves the overall performance of the table search-interpolate subroutines.

Because the two subroutine packages are similar, the text of this document will deal primarily with the differences between EOSPAC and UWEOSPAC. It will describe the calling sequence for each of the subroutines and how to modify the package for including other types of multigroup tables. Where necessary, reference will be made to the EOSPAC document for more information.

2. SESAME EOS Data Files

A SESAME [3] data file is a collection of equations of state (EOS) data tables giving several thermodynamic properties and transport coefficients as functions of material composition, mass density, and temperature. The SESAME data files used by UWEOSPAC are those produced by the MIXERG equation of state and opacity computer code, developed at the University of Wisconsin.

The EOS data table types in each SESAME data file are identified by catalog numbers and are organized into groups called categories. There are four SESAME data categories:

- category 1 contains thermodynamic properties
- category 2 contains photon transport coefficients
- category 3 contains electron transport coefficients
- category 4 contains multigroup transport coefficients.

Category 4 is a new category for SESAME data tables and was created for UWEOSPAC. Thus category 4 tables cannot be used with EOSPAC.

The catalog numbers associated with categories 1, 2, and 3 can be found in the EOSPAC document. These catalog numbers cannot be used with UWEOSPAC. Only the catalog numbers for category 4 listed below can be used with this package.

List of SESAME data table types used by UWEOSPAC -

<u>catalog</u>	<u>name</u>	<u>category</u>	<u>dependent (independent) variables</u>
702	opacrg	4	alog10 rosseland group opacity (alog10 mass density & alog10 temperature)
705	opacpg	4	alog10 planck group opacity (alog10 mass density & alog10 temperature)

Units used in SESAME Category 4 Data Tables -

mass density	g/cm^3
temperature	eV
opacity	cm^2/g

3. The UWEOSPAC Package

The UWEOSPAC package is a set of FORTRAN subroutines that can be used to access SESAME-formatted multigroup opacity tables produced by the MIXERG equation of state and opacity computer code. It is designed for use in hydrodynamics codes that require multigroup transport data and which run on the San Diego Supercomputing Center Cray-XMP computer. The code itself is derived from the EOSPAC subroutine package; the subroutine names and functions follow this precedent.

The Cray FORTRAN source code is a Cray UPDATE deck which requires the FORTLIB function library and the EOSPAC CAL subroutine binary load modules. These are stored on the SDSC Common File System and can be obtained using the following Cray CTSS commands:

MASS GET 002694/UWEOSPAC/UWEOSPAC	<for source code>
MASS GET 002694/UWEOSPAC/BUW	<for binary module>
MASS GET 002694/UWEOSPAC/BEOS2	<for CAL subr. binary>

3.1 Using UWEOSPAC

As noted above, UWEOSPAC is modeled after the EOSPAC package developed at Los Alamos National Laboratory. Like EOSPAC, UWEOSPAC serves as an interface between hydrodynamics codes running on the Cray computer and SESAME EOS data files. The host code is assumed to deal with a physical problem consisting of zones which are organized into groups called regions. The zones and regions must be indexed with consecutive integers beginning with 1. Each region must contain a single material whose identification numbers are specified for all SESAME EOS data table types used in the problem. All regions must use the same EOS data types and more than one region can contain the same material. The host code specifies a region index, a mass density, and a temperature for each zone.

UWEOSPAC accesses the multigroup data tables in two phases. During the setup phase, the appropriate data tables are read into a table storage area (array) provided by the host code. During the search-interpolate phase, data in the table storage area is used to compute the multigroup data value requested by the host code. The host code also provides a storage area to store the computed values.

The table storage area provided by the host code should be a pointered array. This array should be large enough to accommodate all of the multigroup data tables needed by the host code, since no expansion of this array is done. The array size should be larger than

$$13 * ntables + \sum_i ndens_i + ntemps_i + ngrps_i + ndens_i * ntemps_i * ngrps_i$$

where $i = 1$ to $ntables$ and $ntables$ is the number of multigroup tables used by the host code. $ndens_i$, $ntemps_i$, and $ngrps_i$ are the number of densities, temperatures, and groups in the i th table.

The storage area for computed EOS values should be an array large enough to hold computed values for each zone. If the derivatives of the EOS functions are desired or if gathered EOS values are desired, space should be provided for these as well. The array size for the computed EOS values should be

$$nzons * nvals * ngrps$$

where $nzons$ is the number of zones in the problem, $ngrps$ is the number of group tables used, and $nvals$ has the value

- 1, if only the EOS function value is requested,
- 3, if the EOS function and derivatives values are requested,
- 8, if gathered values are requested and bi-linear interpolation used,
- 12, if gathered values are requested and bi-quadratic interpolation, or
- 20, if gathered values are requested and bi-rational function interpolation is used.

3.2 The UWEOSPAC Controllers

The UWEOSPAC subroutine UW1TABS controls the setup phase and is called by the host code. UW1TABS calls the appropriate subroutines to load the required SESAME data tables into the data storage area. The UWEOSAPC subroutine

UW1VALS controls the search-interpolation phase and is also called by the host code. These subroutines perform the same functions as their EOSPAC counterparts ES1TABS and ES1VALS and are the only two UWEOSPAC subroutines that the host code need ever call.

UW1TABS is called just once in the host code and is called during the problem setup phase. Here the host code passes information to UWEOSPAC about how many and which EOS tables to use, how many regions in the problem, what materials are used, and information about the EOS table storage area. Conversion factors for different physical units can be built into the tables so that the host code does not have to do the conversion. Optionally, UW1TABS can print to a file the SESAME data tables used.

UW1VALS is called for each of the EOS table types to be interpolated and is called as often as needed for updating physical properties with changing densities and/or temperatures in the problem zones. Information passed to UW1VALS includes the name of the EOS function to look up, the mass densities and temperatures at which to interpolate the tables, and information about the storage areas.

Specific subroutine arguments and their meanings are listed on the following pages.

SUBROUTINE UW1TABS (LPRINT, IPRNT, MTYPS, MREGS, INAMS, UCONS, IMIDS, IDTAB,
& MTABS, KTABS, IERRS)

Called by -- host-code problem setup routine.

Externals -- UW2INIT, UW2DATA, UW2UNIT, UW2PRNT.

Purpose -- controls UWEOSPAC utility package setup phase to set up and print
designated eos data tables.

Arguments --

LPRNT	= input	logical .true. if tables are to be printed.
IPRNT	= input	integer unit number or hollerith name of eos print file.
MTYPS	= input	integer number of sesame table types used.
MREGS	= input	integer number of regions in problem.
INAMS	= input	integer array containing hollerith names of sesame table types used.
UCONS	= input	real array containing unit conversion factors for all sesame table types for each table variable (x,y,f).
IMIDS	= input	integer array containing material id numbers for all sesame table types for each region.
IDTAB	= input	integer array containing identifiers for eos table area.
MTABS	= in/out	integer length of eos table area.
KTABS	= in/out	integer pointer to eos table area.
IERRS	= output	integer array containing error indicators for all sesame table types for each region, 00 if there are no errors, 21 if eos table area is not initialized, 22 if table type index is out of bounds, 23 if region index is out of bounds, 31 if data table type is not recognized, 32 if no data library files exist, 33 if material id is not in library, 34 if data table type is not in library.

KTABS is set to point to the EOS table area with the FORTLIB function LOC.
Example: if array EOSTAB is to be used for the storage area, the FORTRAN
statement

KTABS = LOC(EOSTAB)

will assign the correct value to KTABS.

SUBROUTINE UW1VALS (IEOSF, IDRVS, INTRP, KTABS, NZONS, NGRP, IREGS, XVALS,
& YVALS, FVALS, IERR1)

Called by -- host-code physics routines.

Externals -- EXP, UW2FUNC, UW2LOOK, ALOG10, AMAX1, UW2INTP, LOC.

Purpose -- controls UWEOSPAC utility package search-interpolation phase
to compute values of eos function $f(x,y)$ and derivatives with
respect to $\log(x,y)$ or to gather eos data table x,y,f values.

Arguments --

IEOSF	= input	hollerith name of eos function.
IDRVS	= input	hollerith name of derivatives.
INTRP	= input	hollerith name of interpolation.
KTABS	= input	integer pointer to eos table area.
NZONS	= input	integer number of zones being processed.
NGRP	= input	integer number of energy groups in problem.
IREGS	= input	integer vector containing indices of regions.
XVALS	= input	real vector containing x values.
YVALS	= input	real vector containing y values.
FVALS	= output	real eos value area.
IERR1	= output	integer error indicator, 00 if there are no errors, 21 if eos table area is not initialized, 22 if table type index is out of bounds, 23 if region index is out of bounds, 24 if data table is not in eos table area, 25 if derivative is not recognized, 26 if interpolation is not recognized, 31 if data table type is not recognized.

Note: for UWEOSPAC, the only recognized names for the EOS functions are
"opacrg" and "opacpg", which stand for the Rosseland and Planck group
opacities.

3.3 Other UWEOSPAC Subroutines

Ordinarily, there is no reason for the host code to call any UWEOSPAC subroutines other than UWITABS and UW1VALS. As noted above, these controller subroutines call the subroutines necessary to load the appropriate SESAME data tables and interpolate them.

Like the EOSPAC subroutines, the UWEOSPAC routines are organized into four levels distinguished by the information they possess. Level-1 subroutines are the controller subroutines described above. These are called by the host code with enough information to satisfy the requirements of the problem. Level-2 subroutines possess the information necessary to access or modify the EOS table storage area. Level-3 subroutines possess the information necessary to access the SESAME-formatted data files. Level-4 subroutines possess only enough information to perform certain operations on specified data sets. Names of the subroutines have the form UW#xxxx, where UW indicates that the subroutine belongs to UWEOSPAC, # = 1, 2, 3, or 4 according to the subroutine level, and xxxx is a four character mnemonic indicating the operation performed. These mnemonics are the same ones used for the corresponding subroutines in EOSPAC. The UW prefix insures that the UWEOSPAC subroutines will not collide with EOSPAC subroutines used in the same program.

The level-1,2,3, and 4 subroutines are described in more detail in the appendix to this document.

4.0 Modifying the UWEOSPAC Subroutine Package

This section describes the procedures necessary to modify UWEOSPAC to allow for more multigroup EOS data table types.

The UWEOSPAC subroutines can be used for interpolating multigroup tables of phenomena which are functions of three independent variables, and where the third independent variable is given as a range of values. For example, the Rosseland opacity is tabulated as a function of mass density, temperature, and photon energy group number. Each energy group is specified by a range, a lower and upper bound, and the ranges are contiguous over all of the groups. Likewise, any table to be interpolated with UWEOSPAC should be similarly constructed. Data tables to be used should be in the SESAME data file format in a Cray "absolute" file as outlined in the appendix.

As mentioned above, UWEOSPAC interpolates only SESAME category 4 tables. Category 4 table types have corresponding catalog numbers which begin with 700. Each table type should have a unique catalog number. Catalog numbers 702 and 705 are currently used for the Rosseland and Planck multigroup opacities.

Material identification numbers for category 4 should be in the range 30001 to 39999. Typically, the last four digits of a material id number uniquely identify a material; the first digit is the category number minus 1. Each material in a SESAME-formatted data table should have a unique id number.

Within UWEOSPAC, there are two subroutines which need to be modified whenever a new EOS data table type is introduced. UW3NAME, which translates table type names into information for the other subroutines, and UW3HDRS, which sets up table headings for the print table option, both need new information about the new table type.

In UW3NAME, there are two statements which need to be changed when a new table type is added. The PARAMETER statement variable NNAMS is the number of table types recognized by UWEOSPAC, and should be incremented when adding a

table type. This will increase the size of the array IINFO, which stores the table type information. The following DATA statement should also be changed, to reflect the change in the size of array IINFO.

Array IINFOS has the dimensions (7,NNAMS), indicating seven pieces of information for each table type name. The first element is the Hollerith name of the data table type and the second is the name of a linked table type (used for Category 1 tables only) and should be blank. Elements 3 and 4 are the catalog number and category number for the table type. Elements 5, 6, and 7 are indicators for the table base, common logarithm, and function. Elements 2, 5 and 7 are held over from the EOSPAC subroutine ES3NAME and have no real meaning here. Element 6 is the common logarithm indicator and equals 1 if the table added contains the common logarithms of the independent variables and function values, or equals 0 otherwise. Then the data statement should look like

```
DATA ((IINFO(JI,JN), JI = 1, NINFS), JN = 1, NNAMS) /
& "OPACRG ", 702, 4, 0, 1, 1,
& "OPACPG ", 705, 4, 0, 1, 1,
& "newname ", 7??, 4, 0, ?, 1 /
```

where uppercase letters and numbers indicate characters should be typed as shown and lowercase letters and question marks are to be filled in.

In UW3HDRS, a PARAMETER statement and DATA statement should be changed when adding another table type. As in UW3NAME, NNAMS should be incremented to reflect the new number of data table types. Data for array variable IHDRS, initialized in the DATA statement, should look like

```

DATA ((IHDRS(JH,JN), JH = 1, 1+NHDRS), JN = 1, NNAMS) /
& "OPACRG ",
& " F(X,Y) = ROSSELAND GRP. OPACITY (CAT. 4, CM2/G / FCNVT)",
& " X = DENS (G/CM3 / XCNVT)Y = TEMP (EV / YCNVT) ",
& "OPACPG ",
& " F(X,Y) = PLANCK GROUP OPACITY (CAT. 4, CM2/G / FCNVT) ",
& " X = DENS (G/CM3 / XCNVT)Y = TEMP (EV / YCNVT) ",
& "newname ",
& " F(X,Y) = function of newname (category, units / FCNVT)",
& " X = name (units / XCNVT)Y = name (units / YCNVT) " /

```

where again, uppercase letters indicate text to be typed as shown. Note that the first element of IHDRS is the Hollerith name of the data table type. The name should be typed EXACTLY as in subroutine UW3NAME, otherwise it will not be recognized, and the data table cannot be printed.

These should be the only changes to the subroutines needed to incorporate new multigroup data table types into UWEOSPAC. If new tables to be added are not similar to the opacity tables already included, consultation of the EOSPAC document and subroutine source code listing may be necessary.

References

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Acknowledgement

This work was supported by Lawrence Livermore National Laboratory under contract number 9265205. Computing facilities provided by the San Diego Supercomputer Center.

APPENDIX

The remainder of the UWEOSPAC subroutines and their arguments are listed on the next few pages.

SUBROUTINE UW2PTRS (KTABS, IERR2)

Called by -- UW2INIT, UW2INFO, UW2DATA, UW2FUNC.

Externals -- none.

Purpose -- sets pointers to arrays within eos table area.

Arguments --

KTABS = input integer pointer to eos table area.
IERR2 = output integer error indicator,
00 if there are no errors,
21 if eos table area is not initialized.

SUBROUTINE UW2INIT (LLOG1, MTYPS, MREGS, INAMS, UCONS, MTABS, KTABS, IERR2)

Called by -- UW1TABS.

Externals -- ES4XPND, UW2PTRS, UW3NAME.

Purpose -- initializes information arrays within eos table area.

Arguments --

LLOG1 = input logical .true. if sesame category 1 tables are to contain common logs.
MTYPS = input integer number of sesame table types used.
MREGS = input integer number of regions in problem.
INAMS = input integer array containing hollerith names of sesame table types used.
UCONS = input real array containing unit conversion factors for all sesame table types for each table variable (x,y,f).
MTABS = in/out integer length of eos table area.
KTABS = in/out integer pointer to eos table area.
IERR2 = output integer error indicator,
00 if there are no errors,
21 if eos table area is not initialized,
31 if data table type is not recognized.

SUBROUTINE UW2INFO (ITYPE, IREGN, KTABS, INAME, LLOGS, XCNVT, YCNVT, FCNVT,
& MATID, ZNBAR, ANBAR, DENSO, ITFWD, IERR2)

Called by -- UW2DATA, UW2UNIT, UW2PRNT.

Externals -- UW2PTRS.

Purpose -- gets information for eos data table.

Arguments --

ITYPE	= input	integer index of data table type.
IREGN	= input	integer index of region.
KTABS	= input	integer pointer to eos table area.
INAME	= output	hollerith name of data table type.
LLOGS	= output	logical log indicator for data table type.
XCNVT	= output	real unit conversion factor for x values.
YCNVT	= output	real unit conversion factor for y values.
FCNVT	= output	real unit conversion factor for f values.
MATID	= output	integer material id number for data table.
ZNBAR	= output	real mean atomic number for data table.
ANBAR	= output	real mean atomic mass for data table.
DENSO	= output	real normal density for data table.
ITFWD	= output	integer first-word index of data table in tbls array.
IERR2	= output	integer error indicator, 00 if there are no errors, 21 if eos table area is not initialized, 22 if table type index is out of bounds, 23 if region index is out of bounds.

SUBROUTINE UW2DATA (ITYPE, IREGN, MATID, MFILS, IFILS, MTABS, KTABS, MLOAD,
& IERR2)

Called by -- UW1TABS.

Externals -- UW2INFO, UW3NAME, UW3LOAD, ALOG10, AMAX1, UW2PTRS.

Purpose -- sets eos data table x,y,f values.

Arguments --

ITYPE	= input	integer index of data table type.
IREGN	= input	integer index of region.
MATID	= input	integer material id number for data table.
MFILS	= input	integer number of data library files.
IFILS	= input	integer array containing unit numbers or hollerith names of data library files.
MTABS	= in/out	integer length of eos table area.
KTABS	= in/out	integer pointer to eos table area.
MLOAD	= output	integer number of words loaded.
IERR2	= output	integer error indicator, 00 if there are no errors, 21 if eos table area is not initialized, 22 if table type index is out of bounds, 23 if region index is out of bounds, 31 if data table type is not recognized, 32 if no data library files exist, 33 if material id is not in library, 34 if data table type is not in library.

SUBROUTINE UW2UNIT (ITYPE, IREGN, KTABS, IERR2)

Called by -- UW1TABS.

Externals -- UW2INFO, UW3NAME, IFIX, ALOG10, AMAX1, UW4CNVT.

Purpose -- sets units of eos data table x,y,f values.

Arguments --

ITYPE	= input	integer index of data table type.
IREGN	= input	integer index of region.
KTABS	= input	integer pointer to eos table area.
IERR2	= output	integer error indicator, 00 if there are no errors, 21 if eos table area is not initialized, 22 if table type index is out of bounds, 23 if region index is out of bounds, 31 if data table type is not recognized.

SUBROUTINE UW2PRNT (IPRNT, ITYPE, IREGN, KTABS, IERR2)

Called by -- UW1TABS.

Externals -- EXP, CHKLUN, UW2INFO, UW3NAME, UW3HDRS, IFIX, MINO, WRITE.

Purpose -- prints eos data table x,y,f values.

Arguments --

IPRNT	= input	integer unit number or hollerith name of eos print file.
ITYPE	= input	integer index of data table type.
IREGN	= input	integer index of region.
KTABS	= input	integer pointer to eos table area.
IERR2	= output	integer error indicator, 00 if there are no errors, 21 if eos table area is not initialized, 22 if table type index is out of bounds, 23 if region index is out of bounds, 31 if data table type is not recognized.

SUBROUTINE UW2FUNC (IEOSF, IDRVS, INTRP, KTABS, ITYPE, LLOGS, NVALS, IINTP, & IERR2)

Called by -- UW1VALS.

Externals -- UW2PTRS, UW3NAME.

Purpose -- gets information for eos function f(x,y) and derivatives.

Arguments --

IEOSF	= input	hollerith name of eos function.
IDRVS	= input	hollerith name of derivatives.
INTRP	= input	hollerith name of interpolation.
KTABS	= input	integer pointer to eos table area.
ITYPE	= output	integer index of data table type.
LLOGS	= output	logical log indicator for data table type.
NVALS	= output	integer number of eos values to be returned.
IINTP	= output	integer index of interpolation.
IERR2	= output	integer error indicator, 00 if there are no errors, 21 if eos table area is not initialized, 24 if data table is not in eos table area, 25 if derivative is not recognized, 26 if interpolation is not recognized, 31 if data table type is not recognized.

SUBROUTINE UW2LOOK (ITYPE, NZONS, IREGS, IZONE, NSRCH, IERR2)

Called by -- UW1VALS.

Externals -- MINO, LEADZ, MASKVN.

Purpose -- performs vector look ahead in problem mesh to find consecutive zones with same material id number.

Arguments --

ITYPE = input integer index of data table type.
NZONS = input integer number of zones being processed.
IREGS = input integer array containing region indices.
IZONE = in/out integer index of next zone to be processed.
NSRCH = output integer length of search vectors.
IERR2 = output integer error indicator,
00 if there are no errors,
22 if table type index is out of bounds,
23 if region index is out of bounds.

SUBROUTINE UW2INTP (ITYPE, IREGN, NVALS, IINTP, NZONS, NSRCH, NGRP, XVALV,
& YVALV, FVALV)

Called by -- UW1VALS.

Externals -- IFIX, UW4BILN, UW4BIQD, UW4BIRF.

Purpose -- performs vector search-interpolation to compute eos function $f(x,y)$ and derivatives wrt x,y or to gather appropriate eos data table x,y,f values.

Arguments --

ITYPE = input integer index of data table type.
IREGN = input integer index of region.
NVALS = input integer number of eos values to be returned.
IINTP = input integer index of interpolation.
NZONS = input integer number of zones being processed.
NSRCH = input integer length of search vectors.
XVALV = input real search vector containing x values.
YVALV = input real search vector containing y values.
FVALV = output real array containing interpolated values of eos function $f(x,y)$ and derivatives wrt x,y or gathered eos data table x,y,f values.

SUBROUTINE UW3NAME (INAME, ILINK, INUMB, ICATE, IBASE, ILOGS, IFUNC, IERR3)

Called by -- UW2INIT, UW2DATA, UW2UNIT, UW2PRNT, UW2FUNC.

Externals -- none.

Purpose -- translates name into information for data table type.

Arguments --

INAME	= input	hollerith name of data table type.
ILINK	= output	hollerith name of linked data table type.
INUMB	= output	integer catalog number of data table type.
ICATE	= output	integer sesame category of data table type.
IBASE	= output	integer base indicator for data table type.
ILOGS	= output	integer 1 if data table contains common logs.
IFUNC	= output	integer index of eos function in data table.
IERR3	= output	integer error indicator, 00 if there are no errors, 31 if data table type is not recognized.

SUBROUTINE UW3HDRS (INAME, IHFX, IERR3)

Called by -- UW2PRNT.

Externals -- none.

Purpose -- translates name into print headers for data table type.

Arguments --

INAME	= input	hollerith name of data table type.
IHFX	= output	hollerith array containing f(x,y) headers.
IERR3	= output	integer error indicator, 00 if there are no errors, 31 if data table type is not recognized.

SUBROUTINE UW3LOAD (MATID, INUMB, MFILS, IFILS, ITABS, MTABS, KTABS, MLOAD,
& IERR3)

Called by -- UW2DATA.

Externals -- GETLEV, FEXIST, CHKLUN, ASSIGN, GETFLEV, RDISK, UNIT, IFIX,
CLOSE.

Purpose -- locates and loads designated data table from sesame data files
into eos table area.

Arguments --

MATID = input integer material id number for data table.
INUMB = input integer catalog number of data table type.
MFILS = input integer number of data library files.
IFILS = input integer array containing unit numbers or hollerith names
of data library files.
ITABS = input integer current index of eos table area.
MTABS = in/out integer length of eos table area.
KTABS = in/out integer pointer to eos table area.
MLOAD = output integer number of words loaded.
IERR3 = output integer error indicator,
00 if there are no errors,
32 if no data library files exist,
33 if material id is not in library,
34 if data table type is not in library.

SUBROUTINE UW4CNVT (LLOGS, XCNVT, YCNVT, FCNVT, NXTBL, NYTBL, NGRP, XTBLs,
& YTBLS, FTBLS)

Called by -- UW2UNIT.

Externals -- none.

Purpose -- converts units of eos data table x,y,f values.

Arguments --

LLOGS = input logical .true. if table contains common logs.
XCNVT = input real unit conversion factor for x values.
YCNVT = input real unit conversion factor for y values.
FCNVT = input real unit conversion factor for f values.
NXTBL = input integer number of data table x values.
NYTBL = input integer number of data table y values.
NGRP = input integer number of photon energy groups.
XTBLS = in/out real array containing data table x values.
YTBLS = in/out real array containing data table y values.
FTBLS = in/out real array containing data table f values.

SUBROUTINE UW4LINE (NVALS, NZONS, NSRCH, NXTBL, NYTBL, NGRP, IXTBL, YTBLS,
& FTBLS, YVALV, FVALV)

Called by -- UW4BILN.

Externals -- SRCHDF, MAX0, MIN0.

Purpose -- performs vector uni-linear (2-point) search-interpolation on eos function $f(x,y)$ holding x fixed. Uses linear extrapolation. 3-dimensional tables are interpolated at each value of the third dimension (ngrp)

Arguments --

NVALS	= in/out	integer number of eos values to be returned.
NZONS	= input	integer number of zones being processed.
NSRCH	= input	integer length of search vectors.
NXTBL	= input	integer number of data table x values.
NYTBL	= input	integer number of data table y values.
NGRP	= input	integer number of photon energy groups.
IXTBL	= input	integer index of data table x value.
YTBLS	= input	real array containing data table y values.
FTBLS	= input	real array containing data table f values.
YVALV	= input	real search vector containing y values.
FVALV	= output	real array containing interpolated values of eos function $f(x,y)$ and derivative wrt y or gathered eos data table y, f values.

SUBROUTINE UW4BILN (NVALS, NZONS, NSRCH, NXTBL, NYTBL, NGRP, XTBL, YTBLS,
& FTBLS, XVALV, YVALV, FVALV)

Called by -- UW2INTP.

Externals -- UW4LINE, SRCHDF.

Purpose -- performs vector bi-linear (4-point) search-interpolation on eos function $f(x,y)$. Uses linear extrapolation. 3-dimensional tables are interpolated at each value of the third dimension (ngrp).

Arguments --

NVALS	= in/out	integer number of eos values to be returned.
NZONS	= input	integer number of zones being processed.
NSRCH	= input	integer length of search vectors.
NXTBL	= input	integer number of data table x values.
NYTBL	= input	integer number of data table y values.
NGRP	= input	integer number of photon energy groups.
XTBLS	= input	real array containing data table x values.
YTBLS	= input	real array containing data table y values.
FTBLS	= input	real array containing data table f values.
XVALV	= input	real search vector containing x values.
YVALV	= input	real search vector containing y values.
FVALV	= output	real array containing interpolated values of eos function $f(x,y)$ and derivatives wrt x,y or gathered eos data table x,y, f values.

SUBROUTINE UW4QUAD (NVALS, NZONS, NSRCH, NXTBL, NYTBL, NGRP, IXTBL, YTBLS,
& FTBLS, YVALV, FVALV)

Called by -- UW4BIQD.

Externals -- SRCH2D, MAX0, MIN0.

Purpose -- performs vector uni-quadratic (3-point) search-interpolation on
eos function $f(x,y)$ holding x fixed. uses linear extrapolation.
3 dimensional tables are interpolated at each value of the third
dimension (ngrp)

Arguments --

NVALS	= in/out	integer number of eos values to be returned.
NZONS	= input	integer number of zones being processed.
NSRCH	= input	integer length of search vectors.
NXTBL	= input	integer number of data table x values.
NYTBL	= input	integer number of data table y values.
NGRP	= input	integer number of photon energy groups.
IXTBL	= input	integer index of data table x value.
YTBLS	= input	real array containing data table y values.
FTBLS	= input	real array containing data table f values.
YVALV	= input	real search vector containing y values.
FVALV	= output	real array containing interpolated values of eos function $f(x,y)$ and derivative wrt y or gathered eos data table y, f values.

SUBROUTINE UW4BIQD (NVALS, NZONS, NSRCH, NXTBL, NYTBL, NGRP, XTBL, YTBLS,
& FTBLS, XVALV, YVALV, FVALV)

Called by -- UW2INTP.

Externals -- UW4QUAD, SRCH2D.

Purpose -- performs vector bi-quadratic (6-point) search-interpolation on
eos function $f(x,y)$. Uses linear extrapolation. 3 dimensional
tables are interpolated at each value of the third dimension
(ngrp).

Arguments --

NVALS	= in/out	integer number of eos values to be returned.
NZONS	= input	integer number of zones being processed.
NSRCH	= input	integer length of search vectors.
NXTBL	= input	integer number of data table x values.
NYTBL	= input	integer number of data table y values.
NGRP	= input	integer number of photon energy groups.
XTBLS	= input	real array containing data table x values.
YTBLS	= input	real array containing data table y values.
FTBLS	= input	real array containing data table f values.
XVALV	= input	real search vector containing x values.
YVALV	= input	real search vector containing y values.
FVALV	= output	real array containing interpolated values of eos function $f(x,y)$ and derivatives wrt x,y or gathered eos data table x,y, f values.

SUBROUTINE UW4RATF (NVALS, NZONS, NSRCH, NXTBL, NYTBL, NGRP, IXTBL, YTBLS,
& FTBLS, YVALV, FVALV)

Called by -- UW4INVT, UW4MERG, UW4BIRF.

Externals -- SRCH3D, MAX0, MIN0, AMIN1, AMAX1, ABS.

Purpose -- performs vector uni-rational-function (4-point) search-interpolation on eos function $f(x,y)$ holding x fixed. uses linear extrapolation. 3 dimensional tables are interpolated at each value of the third dimension (ngrp)

Arguments --

NVALS	= in/out	integer number of eos values to be returned.
NZONS	= input	integer number of zones being processed.
NSRCH	= input	integer length of search vectors.
NXTBL	= input	integer number of data table x values.
NYTBL	= input	integer number of data table y values.
NGRP	= input	integer number of photon energy groups.
IXTBL	= input	integer index of data table x value.
YTBLS	= input	real array containing data table y values.
FTBLS	= input	real array containing data table f values.
YVALV	= input	real search vector containing y values.
FVALV	= output	real array containing interpolated values of eos function $f(x,y)$ and derivative wrt y or gathered eos data table y, f values.

SUBROUTINE UW4BIRF (NVALS, NZONS, NSRCH, NXTBL, NYTBL, NGRP, XTBL, YTBLS,
& FTBLS, XVALV, YVALV, FVALV)

Called by -- UW2INTP.

Externals -- UW4RATF, SRCH3D, AMIN1, AMAX1, ABS.

Purpose -- performs vector bi-rational-function (12-point) search-interpolation on eos function $f(x,y)$. uses linear extrapolation. 3 dimensional tables are interpolated at each value of the third dimension (ngrp)

Arguments --

NVALS	= in/out	integer number of eos values to be returned.
NZONS	= input	integer number of zones being processed.
NSRCH	= input	integer length of search vectors.
NXTBL	= input	integer number of data table x values.
NYTBL	= input	integer number of data table y values.
NGRP	= input	integer number of photon energy groups.
XTBLS	= input	real array containing data table x values.
YTBLS	= input	real array containing data table y values.
FTBLS	= input	real array containing data table f values.
XVALV	= input	real search vector containing x values.
YVALV	= input	real search vector containing y values.
FVALV	= output	real array containing interpolated values of eos function $f(x,y)$ and derivatives wrt x,y or gathered eos data table x,y, f values.

Structure of SESAME Data Files

SESAME data files contain data tabulations of physical properties for various materials. Each file begins with a master directory which contains information about material directories which describe the data tables stored for each material in the file. The contents of these directories are listed below.

Contents of Master Directory (all words type real)

<u>Word</u>	<u>Description</u>
1	number of materials in file (nmats).
2-3	date & version number.
next nmats words	material identification numbers.
next nmats words	lengths of material directories.
next nmats words	pointers to material directories.

Contents of Material Directory (all words type real)

<u>Word</u>	<u>Description</u>
1	material identification number.
2-4	miscellaneous.
5	number of data tables for material (ntbls).
next ntbls words	catalog numbers of data table types stored.
next ntbls words	lengths of data tables stored.
next ntbls words	zero-word indices of data tables stored.

In the above descriptions, lengths are the number of 64-bit words the directory or table occupies in memory, pointers are the number of words past the start of the data file, and zero-word indices are the number of words past the start of the material directory.

After each material directory, the next items listed in the SESAME data file are the basic data table and the EOS data tables. The basic data table is always five words long, but the EOS tables are of variable length, depending on table category number and number of data points tabulated. The contents of the basic data table and EOS tables are listed below.

Contents of Basic Data Table (all words type real)

<u>Word</u>	<u>Description</u>
1	mean atomic number (znbar).
2	mean atomic mass (anbar).
3	normal density (dens0).
4	normal bulk modulus (bmod0).
5	exchange coefficient (xcoef).

Contents of EOS Data Table (all words type real)

<u>Word</u>	<u>Description</u>
1	number of densities (ndens).
2	number of temperatures (ntemps).
next ndens words	densities where data is tabulated.
next ntemps words	temperatures where data is tabulated.
next ndens*ntemps words	EOS data values (density index faster).
next ndens*ntemps words	2nd EOS data values (category 1 tables).

Contents of EOS Category 4 Table (all words type real)

<u>Word</u>	<u>Description</u>
1	number of densities (ndens).
2	number of temperatures (ntemps).
3	number of groups (ngrp).
next ndens words	densities where data is tabulated.
next ntemps words	temperatures where data is tabulated.
next ngrp+1 words	group boundary energies.
next ndens*ntemps*ngrp	EOS data values, density index fastest, temperature index next fastest.