Enhancements for Version 1.1 of ALADDIN

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At the last data center meeting a number of proposals were made for improvements to the first version, 1.0, of ALADDIN distributed by the A+M Data Unit. The scope of the improvements was defined in the presentation of Dr. Hulse, "Future Development of the ALADDIN system", which was presented at the last Data Centre Network meeting. The two basic areas for improvements are:

1. Functional Changes to ALADDIN

   These can be summarized as:

   a) Inclusion of searching procedure for numeric values and the introduction characters in search labels.
   b) The re-introduction of the "Ev" command to generate simple tables of values on linear or logarithmic grids from evaluation function. The current "Ev" command which generates linearly interpolable tables was to be redefined as a new "LT" command.
   c) Specification of non-standard access label "$D" for entries containing coefficients in double precision.
   d) Modification of the output format for table of values generated from the "Ev" and "LT" command.

2. Provision of Labelling Schemes and Dictionaries for Classification of Spectroscopic and Surface Interaction Data

   a) For large data sets or bases of spectroscopic data a scheme for classification and labelling has been defined by Dr. Clark, and this scheme provides for a consistent format for indexing the basic configurations, terms and levels which can then be reffered scheme has been used to store an extensive database for atomic structure and collisional data for photon and electron collision, including a complete database for e^- and hv collisions with all ionization stage of Ti.
   b) A labelling scheme for the classification of surface interaction data was presented at the last data centre meeting from proposals of Janev and Thomas. This format has been used to store and work with sputtering and reflection data in the IAEA A+M data unit.

Searching

- Add search on numerical value of a label in addition to character string match
  - necessary for searching continuous variables used as hierarchical labels, such as wavelengths, energies, etc.
  - new search will work on any hierarchical labels which are "clean" numbers without added characters, etc.
  - search "label" construct will test for a numeric match over a range between values a and b

    =a,b match hierarchical label value between values a and b

  - logical defaults for common special cases

    =a equal to a
    =,b less than or equal to b
    =a, greater than or equal to a

  - non-numeric labels will just give "no match", not an error
- Add substring single character wild card (ABCD?FGH)

Define access label $D to flag double precision coefficients as a special coefficient data field

- Use ALDPCF instead of ALRECF to convert the coefficient field
- Values read into new double precision coefficient array DCF rather usual single precision array CF
- Fitting function routines for double precision fits should use double precision only for coefficients
  - no physical quantity known well enough to require double precision
- Modify ALEV1D to have both CF and DCF arrays, use of DCF flagged by $D
- $D also acts as flag also to allow printout format to be altered for double precision values
  - remove FEXTN flag added to IAEA v1.0

```
C                ********************************
C                * ALTAB AND SUPPORTING ROUTINES *
C                ********************************
C  ..... ..........................................................
C-----    BLOCK FOR EVALUATION FUNCTIONS WITH NON-BLANK (EXCLUDING '$D')
C-----                      ACCESS LABELS.
C
C     FOR ALL EVALUATION FUNCTIONS WITH NON STANDARD ACCESS LABELS
C     (EXCLUDING THE SPECIAL '$D' ACCESS LABEL), THE CALL TO THE ROUTINE
C     FOR HANDLING THE INTERACTIVE DIALOG MUST BE INCLUDED IN THE
C
      IF (BL(NBL) .EQ. '#'.AND. BL(1) .EQ. '$TABSPY') THEN
        CALL RTABSPY
      ELSE
C
C-----      BLOCK FOR EVALUATION FUNCTIONS WITH BLANK AND '$D'
C-----                      ACCESS LABELS.
C
C     FOR ALL EVALUATION FUNCTIONS WITH BLANK ACCESS LABELS (SINGLE
C     PRECISION COEFFICIENTS) OR '$D' ACCESS LABEL (DOUBLE PRECISION
C     COEFFICIENTS) READ THE APROPRIATE COEFFICIENTS INTO ARARAY CF
C     OR DCF.
C
C       RETREIVE NUMERIC COEFFICIENTS FOR THIS FUNCTION THE COEFFICIENTS
C       ARE SINGLE PRECISON NUMBERS
C
        IF(BL(1) .EQ. '$') THEN
          CALL ALRECF(CF, NCF, NCFMX, ERRMSG)
          NDCF = 0
        ELSE IF(BL(1) .EQ. '$D') THEN
          CALL ALDPCF(DCF, NDCF, NCFMX, ERRMSG)
          NCF = 0
C
          ELSE
C
C          CATCH-ALL ENTRIES WITH NON-BLANK OR NON-'$D' ACCESS LABELS
C
           WRITE(LUTOUT,
     &       '(/'' ERROR - ACESS LABEL MUST BE BLANK OR ''$D'' '')')
           RETURN
          ENDIF
C
        IF (ERRMSG .NE.  ' ') THEN
          WRITE(LUTOUT, '(/1X,A)') ERRMSG
          RETURN
        ENDIF

C       RETREIVE NUMERIC COEFFICIENTS FOR THE FUNCTION. THE COEFFICIENTS
C       ARE SINGLE PRECISON NUMBERS
C
         IF(BL(NBL) .EQ. '#MEWE') THEN
          CALL RMEWE
C------
         ELSE IF(BL(NBL) .EQ. '#BELI') THEN
          CALL RBELI
C------
         ELSE IF(BL(NBL) .EQ. '#CHEB') THEN
          CALL RCHEB
    ..............................................
    ..............................................
C------
        ELSE IF(BL(NBL) .EQ. '#TAB1D') THEN
          CALL RTAB1D
C------
```

Example of Subroutine to Control the Handling of an Interactive Dialog for Evaluation Function ALCHEB.

```
C
C#####################################################################
C
      SUBROUTINE RCHEB
C
      EXTERNAL ALCHEB
C
      INCLUDE 'ALPCOM.FOR'
C
      INCLUDE 'ALCOM.FOR'
C
      LOGICAL ALCIEQ
      EXTERNAL ALCIEQ
      DIMENSION XRANGE(10)
C
      WRITE(LUTOUT, '(/'' ORNL:CFADC CHEBYSHEV POLYNOMIAL FIT'')' )
C
C      CHECK NUMBER OF SINGLE PRECISION COEFFICIENTS
C
      IF(NCF .NE. 11) THEN
        WRITE(LUTOUT, '(/'' INCORRECT NUMBER OF COEFFICIENTS )'')')
        RETURN
      ENDIF
      WRITE(LUTOUT, '(/'' (INPUT VALID RANGE FROM'',
     &     1PE10.2, '' TO'', 1PE10.2, '')'')' ) CF(10), CF(11)
C
C      INCLUDE CODING TO CHOICE BETWEEN TABLE OUTPUT TYPES
C
      IF(ALCIEQ(CMND(1:2),'EV')) THEN
        CALL ALEV1D(ALCHEB)
      ELSE
        CALL ALREVD(PERUNC,XRANGE(1),XRANGE(2))
        IF (PERUNC .EQ. 0.0) RETURN
        NRANGE=1
C
        CALL ALTB1D(PERUNC,ALCHEB,NRANGE,XRANGE)
C
      ENDIF
C
      RETURN
```

```
      SUBROUTINE ALCHEB(PET, PCF, KNCF, PDCF, KNDCF, PFIT, KERMSG)
C
C     THIS IS AN ORNL:CFADC SUBROUTINE TO CALCULATE CROSS SECTIONS IN
C     (cm[2]) VERSUS ENERGY IN (EV/AMU) OR RATE COEFFICIENTS IN
C     (cm[3]/s) VERSUS MAXWELLIAN TEMPERATURE IN (eV) FROM CHEBYSHEV
C     POLYNOMIAL FITTING COEFFICIENTS
C
C     THESE FITS ARE VALID ONLY BETWEEN THE LIMITS EMIN AND EMAX,
C     WHICH ARE COEFFICIENTS PCF(10) AND PCF(11) IN THE ENTRY DATA FIELD
C
C     PET = COLLISION ENERGY IN eV/amu OR MAXWELLIAN TEMPERATURE IN eV
C
C     KERMSG = BLANK IF NO ERRORS
C
C     PFIT = CROSS SECTION IN cm[2] OR RATE COEFFICIENT IN cm[3]/s
C
C     WRITTEN BY H. HUNTER, CFADC OAK RIDGE NATIONAL LABORATORY
C-----------------------------------------------------------------------
C     SINGLE PRECISION COEFFICIENTS MUST BE SUPPLIED IN ARRAY PCF
C=======================================================================
C
      REAL PET, PCF, PFIT
      REAL EMIN, EMAX, CHEB, EMINL, EMAXL, ENL, XNORM
      REAL TWOX, PREV, PREV2
C
      DOUBLE PRECISION PDCF
      DIMENSION PCF(KNCF), PDCF(KNDCF)
C
      CHARACTER*(*) KERMSG
C
      EMIN = PCF(10)
      EMAX = PCF(11)
      IF(PET .GE. EMIN .AND. PET .LE. EMAX) THEN
        KERMSG = ' '
      ELSE
        KERMSG = 'OUTSIDE RANGE OF FIT IN ALCHEB'
        RETURN
      ENDIF
C
C     CALCULATE POLYNOMIAL USING RECURSION RELATION
C
      K = 9
      CHEB = PCF(K)
      EMINL = LOG(EMIN)
      EMAXL = LOG(EMAX)
      ENL= LOG(PET)
      K = K-1
      XNORM = (ENL-EMINL-(EMAXL-ENL)) / (EMAXL-EMINL)
      TWOX = 2.0 *  XNORM
      PREV2 = 0.0
   10 PREV = CHEB
      IF(K .NE. 1) THEN
        CHEB = PCF(K) + TWOX*PREV - PREV2
        PREV2 = PREV
        K = K-1
        GO TO 10
      ENDIF
      CHEB = 0.5*PCF(1) + XNORM*PREV - PREV2
      PFIT = EXP(CHEB)
  100 RETURN
      END
```

Reinstate original "EV"-style linear / log data points for quick access to data values

- Provides needed fast, simple output of data values at fixed number of points
- Modify file output format slightly or ease of use by other codes
  - ! flags comment lines
  - # flags new line giving number of lines and columns for input "DO" loop
  - * flags line with column headers
  - use evaluation label as data column header
  - setup header for easy copy/paste for Macintosh
- Example of modified format

```
Test ev command output file
!
# 10  2
*          INPUT              #MEWE

 1     1.000000E+00       8.158804E-09
 2     1.111111E+00       7.890224E-09
 3     1.222222E+00       7.652079E-09
 4     1.333333E+00       7.438783E-09
 5     1.444444E+00       7.246118E-09
 6     1.555556E+00       7.070816E-09
 7     1.666667E+00       6.910307E-09
 8     1.777778E+00       6.762531E-09
 9     1.888889E+00       6.625819E-09
10     2.000000E+00       6.498793E-09
```

Table 1. Classes of *PSI collisions

(defined by type of the projectile and state of the surface)

1. e + surface
2. e + adsorbate + surface
3. atom + surface
4. atom + adsorbate + surface
5. Molecule + surface
6. Molecule + adsorbate + surface
7. Photon + surface
8. Photon + adsorbate + surface

In this notation atom (molecule) represents atom (molecule) or atomic (molecular) ion.

Table 2. Categories of PSI processes

(defined by fate of projectile or kind of observed particle)

1. Particle adsorption (sticking) penetration
2. Penetration (Range, Energy Loss)
3. Particle trapping, retention and release (detrapping)
4. Particle desorption (including thermal)
5. Particle backscattering (reflection)
6. Secondary electron emission (particle induced)
7. Sputtering (including physical, physics-chemical, chemical, and enhanced sublimation)
8. Composite PSI processes

* PSI = particle-surface interaction

B. PROCESS LABELS

Table 3. Categorization and Labelling of Particle-Surface Collision Processes

	1.	Class of collision
(*)	2.	Type of collision
(*)	3.a	Chemical symbol of projectile
(*)	3.b	Charge state of projectile
(* *)	3.c	Quantum state of projectile
(*)	4.a	Chemical symbol of target
(*)	4.b	Aggregation state of target
(*)	5.a	Chemical symbol of substrate
(*)	5.b	Aggregation state of substrate
		---------- (collision)
(*)	6.a	Chemical symbol of observed species
(# *)	6.b	Charge state of observed species
(* *)	6.c	Quantum state of observed species
(*)	6.d	Aggregation state of observed species
(*)	7.a	Chemical symbol of target
(*)	7.b	Aggregation state of target

Notes: (1) Labels marked * are mandatory.
(2) Aggregation state is either:
(a) Surface (or solid) - surf.
(b) Adsorbed - ads.
(c) Trapped - trap.
(3) Labels for charged (# *) and quantum states (* *) are added when necessary to specify a particular reaction channel. These should follow the scheme for atomic collision data.
(4) In many cases the charge and quantum state of the observed species may not be known (as for example in total sputtering).
(5) Sections 4 and 5 are both required only if the problem involves one species adsorbed on another. In most cases there is only a single target situation and 5 is omitted.
(6) The post collision situation lists first, as item 6, the observed species, which is not necessarily the projectile. This will differ from the atomic data case.
(7) The final entry 7 is listed only for completeness and is the target material (or substrate underlying an adsorbate). It should be the same as item 4 is an adsorbate). In general item 7 is undefined in the specification of data and is redundant.

(8) Entry 3 is always the incident particle when is a free atom, ion or electron. The entry 6 is always the observed species and this is normally also a free atom, ion or electron.

Table 4. Dictionary of Collision Processes

No.	Process	Abbreviation	Symbolic Notation
	Group A. Binary Processes Leading to Reflection of the Incident Species		
A.1.	Reflection of atoms - total	RAT	A+B(surf)→A+B(surf)
A.2.	Reflection of atoms - specific	RAE	A+B(surf)→A^*+B(surf)
A.3.	Reflection of atoms - specific	RAC	A+B(surf)→A^{k+}+B(surf)
A.4.	Dissociation of molecules and reflection	RMD	AB+C(surf)→A+B+C(surf)
A.5.	Reflection of atoms - energy distribution	RAENER	A+B(surf)→A+B(surf)
A.6.	Reflection of electrons - total	RET	e+B(surf)→e+B(surf)
A.7.	Reflection of electrons - energy distribution	REENER	e+B(surf)→e+B(surf)
	Group B. Binary Processes Leading to Ejection of the Target Species		
B.1.	Sputtering by atoms - total	SAT	A+B(surf)→B+B(surf)
B.2.	Sputtering by atoms leading to specific excited states	SAE	A+B(surf)→B^*+B(surf)
B.3.	Sputtering by atoms leading to specific charge states	SAC	A+B(surf)→B^{k+}+B(surf)
B.4.	Sputtering by atoms - energy distribution	SAENER	A+B(surf)→B+B(surf)
B.5.	Sputtering by electrons	SE	e+B(surf)→B+B(surf)
B.6.	Electron ejection by photons	EEP	hν+B(surf)→e+B(surf)
B.7.	Secondary electron ejection by atoms	SEA	A+B(surf)αe+B(surf)
B.8.	Secondary electron ejection by atoms energy distribution	SEAENER	A+B(surf)→e+B(surf)

4.1.3 Atomic Structure, Radiative Processes and Autoionization Processes

Atomic structure, radiative processes, and autoionization processes are needed in plasma modeling. All of this information is readily incorporated into the ALADDIN system. The hierarchical labeling is summarized in Table 6. The general scheme of labeling is similar to that described above. The inclusion of an integer index for each configuration, LS-term, and fine-structure energy level can be used in place of the full set of quantum numbers both in the radiative processes and in the collisional processes.

TABLE 6

ATOMIC STRUCTURE, RADIATIVE PROCESSES, AND AUTOIONIZATION PROCESSES

No.	Process	Hierarchical Label
S.1	Configuration average energies	CONFIGS
S.2	LS-term energies	TERMS
S.3	Fine Structure Level Energies	LEVELS
R.1	Bound-Bound Radiative Transitions	GF
R.2	Bound-Free Radiative Transitions	PHOTION
AI.1	Autoionization Rates	AUTOION
AI.2	Branching Ratios	BRAT

Table I. Number of configurations, collisional excitations, autoionization states and oscillator strengths calculated for each ion stage.

Ionization Stage	Number of Configurations	Number of Excitations	Number of Autoionizations	Number of gf
1	233	35	1609	1015
2	195	38	1054	834
3	825	59	10278	4950
4	780	59	8511	4698
5	546	50	5128	3141
6	594	54	5279	3546
7	594	54	5017	3575
8	594	54	4867	3575
9	594	54	4610	3575
10	539	54	3650	3180
11	309	44	1615	1602
12	246	47	1176	1262
13	427	36	2051	2460
14	453	38	2439	2715
15	455	38	2430	2730
16	455	38	2408	2730
17	455	38	2314	2730
18	377	38	1811	2190
19	209	26	808	1060
20	119	27	366	596
21	120	14	366	600
22	15	14	0	40

III. Evaluated Atomic Databases

A. A+M Collisional Databases

1. "Atomic and Molecular Data for Fusion, Part I - Recommended Cross Sections and Rates for Electron Ionisation of Light Atoms and Ions," K.L. Bell, H.B. Gilbody, J.G. Hughes, A.E. Kingston and F.J. Smith. J. Phys. Chem. Ref. Data 12, 891 (1983).

2. "Recommended Data on Excitation of Carbon and Oxygen Ions by Electron Collisions," Y. Itikawa, S. Hara, T. Kato, S. Nakazaki, M.S. Pindzola, D.H. Crandall. At. Data Nucl. Data Tables (ADNDT) 33, 149 (1985).

3. "Recommended Data on Atomic Collision Processes Involving Iron and its Ions," C. Bottcher, D.C. Griffin, H.T. Hunter, R.K. Janev, A.E. Kingston, M.A. Lennon, R.A. Phaneuf, M.S. Pindzola, S.M. Younger. Nucl. Fusion, Special Supplement, (1987).

4. "Collisions of Carbon and Oxygen Ions with Electrons, H, H_2 and He". Atomic Data for Controlled Fusion Research, Vol. V. R.A. Phaneuf, R.K. Janev, M.S. Pindzola (Editors). Report ORNL-6090/V5, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, USA (1987).

5. "Atomic and Molecular Data for Fusion, Part II - Recommended Cross Sections and Rates for Electron Ionisation of Light Atoms and Ions: Fluorine to Nickel," M.A. Lennon, K.L. Bell, H.B. Gilbody, J.G. Hughes, A.E. Kingston, M.J. Murray, F.J. Smith. J. Phys. Chem. Ref. Data 17, 1285 (1988).

6. "Recommended Data for Excitation Rate Coefficients of Helim Atoms and Helim-like Ions by Electron Impact," T. Kato and S. Nakazaki. At. Data. Nucl. Data Tables (ADNDT), 42, 313 (1989).

7. "Elementary Processes in Hydrogen-Helium Plasmas", R.K. Janev, W.D. Langer, K. Evans Jr., D.E. Post Jr., Springer-Verlag, (1987).

8. "Collisions of H, H_2, He and Li Atoms and Ions with Atoms and Molecules, Vol. 1. C.F. Barnett, (Editor). Report ORNL-6086/V1, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, USA (1990).

9. "Atomic and Molecular Data for Fusion, Part III. Recommended Cross Sections and Rates for Electron Ionization of Atoms and Ions: Copper to Uranium", M.J. Higgins, M.A. Lennon, J.G. Hughes, K.L. Bell, H.B. Gilbody, A.E. Kingston, F.J. Smith, Culham Report, CLM-R294, Abingdon, Oxfordshire, U.K., (1989).

Note: The above numerical data files are formatted in the ALADDIN database management system. The evaluated data and the ALADDIN system software and mannual are available on request, free of charge, from the IAEA Atomic and Molecular Data Unit. The data files can be provided on high or low density floppy diskettes or magnetic tape. The IAEA is also connected to the EARN-Bitnet network and requests for data can be sent to RNDS@IAEA1.

B. Particle-Surface Interaction Databases

1. "Energy dependence of Ion-Induced Sputtering Yields of Monatomic Solids in the Low Energy Region", N. Matsunami, Y. Yamamura, N. Itoh, H. Tawara, T. Kawamura.
   Report IPPJ-AM-52, Institute of Plasma Physics, Nagoya, Japan (1987).

2. "Energy Dependence of the Yields of Ion-Induced Sputtering of Montatomic Solids", N. Maksunami, Y. Yamaura, Y. Itikawa, N. Itoh, Y. Kazumata, S. Miyagawer, K. Morita, R. Strimizu, H. Tawara.
   Report IPPJ-AM-32, Institute of Plasma Physics, Nagoya, Japan (1988).