ADAS Subroutine c4spln

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      SUBROUTINE C4SPLN( MXBE   , MXTD   , MXTT   , MXREQ  ,
     &                   NREQ   , BMENGA , DENSA  , TIA    ,
     &                   NSITYP , SVREF  , NBE    , BE     ,
     &                   NTDENS , TDENS  , NTTEMP , TTEMP  ,
     &                   SVT    , SVED   , SVREQ  , LIBMA  ,
     &                   LIDNA  , LITIA  , ZEFF   , ITZ    ,
     &                   LSET   )
C
C
C-----------------------------------------------------------------------
C
C  ****************** FORTRAN77 SUBROUTINE: C4SPLN *********************
C
C  PURPOSE: CALCULATES THE BEAM STOPPING COEFFICIENT FOR EACH TRIPLET
C           OF BEAM ENERGY, ION DENSITY AND ION TEMPERATURE. IT USES
C           A ONE-WAY CUBIC SPLINE FOR THE TEMPERATURE AND A TWO-WAY
C           CUBIC SPLINE FOR THE ENERGY/DENSITY PAIR TO DETERMINE THE
C           STOPPING COEFFICIENT FROM THE INPUT DATA SET. IF A VALUE
C           CANNOT BE INTERPOLATED USING SLPINES THEN IT IS
C           EXTRAPOLATED BY 'XXSPLE'.
C
C  CALLING PROGRAM: CXBMS / ADAS304
C
C  SUBROUTINE:
C
C  INPUT : (I*4)  MXBE      = MAXIMUM NUMBER OF BEAM ENERGIES WHICH CAN
C                             BE READ.
C  INPUT : (I*4)  MXTD      = MAXIMUM NUMBER OF TARGET DENSITIES WHICH
C                             CAN BE READ.
C  INPUT : (I*4)  MXTT      = MAXIMUM NUMBER OF TARGET TEMPERATURES
C                             WHICH CAN BE READ.
C  INPUT : (I*4)  MXREQ     = MAXIMUM NUMBER OF REQUESTED TRIPLETS OF
C                             BEAM ENERGY, ION DENSITY AND ION TEMP.
C  INPUT : (I*4)  NREQ      = NUMBER OF REQUESTED TRIPLETS OF BEAM
C                             ENERGY, ION DENSITY AND ION TEMP.
C  INPUT : (R*8)  BMENGA()  = REQUESTED BEAM ENERGIES.
C                             UNITS: EV/AMU
C                             DIMENSION: NREQ
C  INPUT : (R*8)  DENSA()   = REQUESTED ION DENSITIES.
C                             UNITS: CM-3
C                             DIMENSION: NREQ
C  INPUT : (R*8)  TIA()     = REQUESTED ION TEMPERATURES.
C                             UNITS: EV
C                             DIMENSION: NREQ
C  INPUT : (I*4)  NSITYP    = NUMBER OF STOPPING ION TYPES.
C  INPUT : (R*8)  SVREF()   = STOPPING COEFFT. AT REFERENCE BEAM ENERGY,
C                             TARGET DENSITY AND TEMPERATURE.
C                             UNITS: CM3 S-1
C                             DIMENSION: NSITYP
C  INPUT : (I*4)  NBE()     = NUMBER OF BEAM ENERGIES.
C                             DIMENSION: NSITYP
C  INPUT : (R*8)  BE(,)     = BEAM ENERGIES.
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C                                UNITS: EV/AMU
C                                1ST DIMENSION: MXBE
C                                2ND DIMENSION: NSITYP
C  INPUT : (I*4)  NTDENS()   = NUMBER OF TARGET DENSITIES.
C                                DIMENSION: NSITYP
C  INPUT : (R*8)  TDENS(,)   = TARGET DENSITIES.
C                                UNITS: CM-3
C                                1ST DIMENSION: MXTD
C                                2ND DIMENSION: NSITYP
C  INPUT : (I*4)  NTTEMP()   = NUMBER OF TARGET TEMPERATURES.
C                                DIMENSION: NSITYP
C  INPUT : (R*8)  TTEMP(,)   = TARGET TEMPERATURES.
C                                UNITS: EV
C                                1ST DIMENSION: MXTT
C                                2ND DIMENSION: NSITYP
C  INPUT : (R*8)  SVT(,)     = STOPPING COEFFT. AT REFERENCE BEAM ENERGY
C                                AND TARGET DENSITY.
C                                UNITS: CM3 S-1
C                                1ST DIMENSION: MXTT
C                                2ND DIMENSION: NSITYP
C  INPUT : (R*8)  SVED(,,)   = STOPPING COEFFT. AT REFERENCE TARGET
C                                TEMPERATURE.
C                                UNITS: CM3 S-1
C                                1ST DIMENSION: MXBE
C                                2ND DIMENSION: MXTD
C                                3RD DIMENSION: NSITYP
C  OUTPUT: (R*8)  SVREQ(,)   = STOPPING COEFFT. AT REQUESTED BEAM ENERGY,
C                                ION DENSITY AND ION TEMPERATURE.
C                                UNITS: CM3 S-1
C                                1ST DIMENSION: MXREQ
C                                2ND DIMENSION: NSITYP
C  OUTPUT: (L*4)  LIBMA(,)   = FLAGS IF INTERPOLATION OR EXTRAPOLATION
C                                USED FOR REQUESTED BEAM ENERGIES.
C                                .TRUE.  => INTERPOLATION USED.
C                                .FALSE. => EXTRAPOLATION USED.
C                                1ST DIMENSION: MXREQ
C                                2ND DIMENSION: NSITYP
C  OUTPUT: (L*4)  LIDNA(,)   = FLAGS IF INTERPOLATION OR EXTRAPOLATION
C                                USED FOR REQUESTED ION DENSITIES.
C                                .TRUE.  => INTERPOLATION USED.
C                                .FALSE. => EXTRAPOLATION USED.
C                                1ST DIMENSION: MXREQ
C                                2ND DIMENSION: NSITYP
C  OUTPUT: (L*4)  LITIA(,)   = FLAGS IF INTERPOLATION OR EXTRAPOLATION
C                                USED FOR REQUESTED ION TEMPERATURES.
C                                .TRUE.  => INTERPOLATION USED.
C                                .FALSE. => EXTRAPOLATION USED.
C                                1ST DIMENSION: MXREQ
C                                2ND DIMENSION: NSITYP
C  INPUT:  (R*8)  ZEFF()     = USED AS A WEIGHTING FACTOR ASSOCIATED
C                                WITH THE EVALUATION OF AN EFFECTIVE
C                                DENSITY.
C  INPUT:  (I*4)  ITZ()      = ARRAY CONTAINING THE NUCLEAR CHARGE OF
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C       EACH IMPURITY CONSIDERED.
C  INPUT:  (L)    LSET      = LOGICAL FLAGGING WHETHER OR NOT THE INPUT
C                             DATASET VECTOR HAS CHANGED. IF SO, A
C                             REQUEST TO REDO THE SPLINES IS PASSED TO
C                             'XXSPLF'.
C
C  PARAM : (I*4)  MXI       = MAX. NO. OF STOPPING ION TYPES >= NSITYP.
C  PARAM : (I*4)  MXIN      = MAX. NO. OF INPUT DATA SET VALUES
C                             >= MXBE , MXTD , MXTT.
C  PARAM : (I*4)  MXOUT     = MAX. NO. OF OUTPUT VALUES >= NREQ.
C
C          (I*4)  IOPT      = DEFINES THE BOUNDARY DERIVATIVES FOR THE
C                             SPLINE ROUTINE 'XXSPLE'. SEE 'XXSPLE'.
C                             ( VALID VALUES = <0, 0, 1, 2, 3, 4)
C          (I*4)  NOUT      = NUMBER OF OUTPUT VALUES FOR SPLINE.
C          (I*4)  I         = LOOP INDEX.
C          (I*4)  J         = LOOP INDEX.
C          (I*4)  K         = LOOP INDEX.
C
C          (L*4)  LSETX     = FLAGS TO SPLINE ROUTINE 'XXSPLF' IF
C                             'X' SPLINE PARAMETERS SHOULD BE SET UP.
C                             .TRUE.  => SET UP SPLINE PARAMS.
C                             .FALSE. => DO NOT SET UP SPLINE PARAMS.
C          (L*4)  LSETY     = FLAGS TO SPLINE ROUTINE 'XXSPLE' IF
C                             'Y' SPLINE PARAMETERS SHOULD BE SET UP.
C                             .TRUE.  => SET UP SPLINE PARAMS.
C                             .FALSE. => DO NOT SET UP SPLINE PARAMS.
C
C          (R*8)  DYT(,)    = DERIVATIVES FOR SPLINE INTERPOLATION OVER
C                             TEMPERATURE. ONE VECTOR FOR EACH TARGET
C                             ION.  SAVED FOR SPEED ON MULTIPLE CALLS
C                             DIMENSION: (MXIN,MXI)
C          (R*8)  QT(,)     = SPLINE INTERPOLATED SECOND DERIVATIVES.
C          (R*8)  D1T(,)    = MULTIPLICATION FACTOR USED IN XXSPLF.
C          (R*8)  D2T(,)    = MULTIPLICATION FACTOR USED IN XXSPLF.
C          (R*8)  D3T(,)    = MULTIPLICATION FACTOR USED IN XXSPLF.
C          (R*8)  DYE(,,)   = DERIVATIVES FOR SPLINE INTERPOLATION OVER
C                             ENERGY. ONE VECTOR FOR EACH INPUT ENERGY
C                             AND TARGET ION.  SAVED FOR SPEED ON
C                             MULTIPLE CALLS
C                             DIMENSION: (MXIN,MXIN,MXI)
C          (R*8)  QE(,)     = SPLINE INTERPOLATED SECOND DERIVATIVES.
C          (R*8)  D1E(,)    = MULTIPLICATION FACTOR USED IN XXSPLF.
C          (R*8)  D2E(,)    = MULTIPLICATION FACTOR USED IN XXSPLF.
C          (R*8)  D3E(,)    = MULTIPLICATION FACTOR USED IN XXSPLF.
C          (R*8)  DYD(,)    = DERIVATIVES FOR SPLINE INTERPOLATION OVER
C                             DENSITY. ONE VECTOR FOR EACH TARGET ION.
C                             SAVED FOR SPEED ON MULTIPLE CALLS
C                             DIMENSION: (MXIN,MXI)
C          (R*8)  QD(,)     = SPLINE INTERPOLATED SECOND DERIVATIVES.
C          (R*8)  D1D(,)    = MULTIPLICATION FACTOR USED IN XXSPLF.
C          (R*8)  D2D(,)    = MULTIPLICATION FACTOR USED IN XXSPLF.
C          (R*8)  D3D(,)    = MULTIPLICATION FACTOR USED IN XXSPLF.
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C
C          (R*8)  YOUT()     = Y OUTPUT ARRAY FROM SPLINE ROUTINE.
C                              DIMENSION: MXOUT
C
C          (R*8)  SVTO(,)    = STOPPING COEFFICIENTS AT REQUESTED ION
C                              TEMPERATURES.
C                              1ST DIMENSION: MXOUT
C                              2ND DIMENSION: MXI
C          (R*8)  SVEDO(,)   = STOPPING COEFFICIENTS AT REQUESTED BEAM
C                              ENERGIES AND ION DENSITY.
C                              1ST DIMENSION: MXOUT
C                              2ND DIMENSION: MXI
C          (R*8)  YPASS(,)   = STOPPING COEFFICIENTS AT REQUESTED BEAM
C                              ENERGIES.
C                              1ST DIMENSION: MXIN
C                              2ND DIMENSION: MXOUT
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          ------------------------------------------------------------
C          I4UNIT     ADAS      RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C          XXSPLF     ADAS      SPLINE SUBROUTINE (EXTENDED DIAGNOSTICS)
C          R8FUN1     ADAS      PERFORMS TRANSFORMATION ( X -> X )
C
C AUTHOR:  JONATHAN NASH  (TESSELLA SUPPORT SERVICES PLC)
C          K1/0/87
C          JET EXT. 5183
C
C DATE:    10/12/93
C
C UNIX-IDL PORT:
C
C VERSION: 1.1                          DATE: 16-11-95
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C               - FIRST VERSION
C VERSION: 1.2
C MODIFIED: HARVEY ANDERSON
C    - THE BEAM STOPPING COEFFICIENT FOR EACH
C   INDIVIDUAL IMPURITY WAS BEING EVALUATED
C   AT THE WRONG DENSITY. THE BEAM STOPPING
C   COEFFICIENT SHOULD BE EVALUATED AT AN
C   EFFECTIVE DENSITY. THIS HAS BEEN CORRECTED.
C - THE TARGET DENSITY READ FROM ADF21 FILE IS THE
C   ELECTRON DENSITY. THE CORRECTION TO THE EVALUATION
C   OF THE EFFECTIVE DENSITY WAS DONE IN TERMS OF THE
C   ION DENSITY. THIS WAS CORRECTED SO THAT THE EFFECTIVE
C   DENSITY IS EVALUATED IN TERMS OF THE ELECTRON DENSITY.
C   20/12/96
C - INTRODUCED THE PARAMETER FACT2, TO ENABLE THE
C   EFFECTIVE ELECTRON DENSITY TO BE EVALUATED.ORIGINALY
C   THE USER WOULD ENTER THE TOTAL ION DENSITY AND
C   THE STOPPING COEFFICIENTS WOULD BE EVALUATED AT AN
C   EFFECTIVE ELECTRON DENSITY. NOW THE CODE HAS BEEN
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C   CHANGED TO ALLOW THE USER TO ENTER THE TOTAL ELECTRON
C   DENSITY.
C
C VERSION: 1.3                          DATE: 19-03-03
C MODIFIED: LORNE HORTON
C               - INCREASED MXOUT TO ALLOW UP TO 1024 EVALUATIONS PER
C                 CALL.
C               - IMPLEMENTED XXSPLF TO SPEED BICUBIC SPLINING BY
C                 HOLDING AS MUCH AS POSSIBLE IN GLOBAL VARIABLES.
C               - REPLACED FACT1 AND FACT2 WITH ZEFF
C
C-----------------------------------------------------------------------
C
C-----------------------------------------------------------------------
      INTEGER             ITZ(NSITYP), MXBE,        MXREQ,       MXTD
      INTEGER             MXTT,        NBE(NSITYP), NREQ,        NSITYP
      INTEGER             NTDENS(NSITYP),           NTTEMP(NSITYP)
      LOGICAL             LIBMA(MXREQ,NSITYP),      LIDNA(MXREQ,NSITYP)
      LOGICAL             LITIA(MXREQ,NSITYP),      LSET
      REAL*8              BE(MXBE,NSITYP),          BMENGA(NREQ)
      REAL*8              DENSA(NREQ), SVED(MXBE,MXTD,NSITYP)
      REAL*8              SVREF(NSITYP),            SVREQ(MXREQ,NSITYP)
      REAL*8              SVT(MXTT,NSITYP),         TDENS(MXTD,NSITYP)
      REAL*8              TIA(NREQ),   TTEMP(MXTT,NSITYP)
      REAL*8              ZEFF(NREQ)
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