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INTERNATIONAL ATOMIC ENERGY AGENCY

NUCLEAR DATA SERVICES

DOCUMENTATION SERIES OF THE IAEA NUCLEAR DATA SECTION

Implementing and Testing the LINTAB, HEATER and PLOTTAB code package

Dermott E. Cullen and James J. Smith

Abstract: Enclosed is a describtion of the magnetic tape or floppy diskette containing the LINTAB, HEATER and PLOTTAB code package. In addition detailed information is provided on implementation and testing of these codes. These codes are documented in IAEA-NDS-84.

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SUMMARY OF THE ATOMIC AND MOLECULAR DATA SUPPORT PACKAGE (VERSION 87-1)

PURPOSE

THIS SET OF PROGRAMS IS DESIGNED TO CALCULATE AND PLOT ATOMIC AND MOLECULAR CROSS SECTIONS AND REACTION RATES.

GRAPHICS INTERFACE

PROGRAM PLOTTAB USES A SIMPLE CALCOMP LIKE GRAPHICS INTERFACE WHICH REQUIRES ONLY 3 SUBROUTINES...PLOTS, PLOT AND PEN (DESCRIBED IN THE PROGRAM DOCUMENTATION). ALL CHARACTERS AND SYMBOLS ARE DRAWN USING TABLES OF PEN STROKES (SUPPLIED WITH THIS PROGRAM). USING THIS METHOD THE PROGRAM SHOULD BE SIMPLE TO INTERFACE TO VIRTUALLY ANY PLOTTER OR GRAPHICS TERMINAL AND THE APPEARANCE AND LAYOUT OF THE PLOTS SHOULD BE INDEPENDENT OF WHICH PLOTTER IS USED.

CODE	VERSION	CPU TIME	CORE (KILO BYTES)	PURPOSE
LINTAB	87-1	0.02	211	STARTING FROM A MODEL CACULATE LINEARLY INTERPOLABLE TABULATED CROSS SECTIONS.
HEATER	87-1	0.53	288	STARTING FROM LINEARLY INTERPOLABLE TABULATED CROSS SECTIONS (I.E., LINTAB OUTPUT) CALCULATE REACTION RATES IN LINEARLY INTERPOLABLE TABULATED FORM.
PLOTTAB	87-2	0.09	456	STARTING FROM LINEARLY INTERPOLABLE TABULATED DATA AND/OR EXPERIMENTALLY MEASURED POINTS (I.E., LINTAB OR HEATER OUTPUT) PLOT A COMPARISON OF UP TO 30 SETS OF TABLES AND/OR SETS OF DISCRETE POINTS.

CPU TIME = IBM-3083 CPU MINUTES FOR ENCLOSED EXAMPLE PROBLEM.
CORE = IBM FORTRAN-77 COMPILER

COMPUTERS ON WHICH PROGRAM WILL OPERATE

THESE PROGRAMS ARE DESIGNED TO OPERATE ON VIRTUALLY ANY TYPE OF COMPUTER FROM LARGE MAINFRAMES ALL THE WAY DOWN TO AN IBM-PC-AT. THE REMAINDER OF THIS REPORT DESCRIBES THE PROGRAMS AS IMPLEMENTED ON A MAINFRAME COMPUTER. CONTACT THE AUTHOR IF YOU WISH TO OBTAIN A COPY OF THESE PROGRAMS ON DISKETTES FOR USE ON AN IBM-PC-AT (WARNING...THESE PROGRAMS ON DISKETTES ARE ONLY DISTRIBUTED ON 1.2 MEGABYTE DISKETTES WHICH CAN ONLY BE USED ON A PC WITH 1.2 MEGABYTE DISK DRIVES, E.G. AN IBM-PC-AT. PLEASE DO NOT REQUEST THESE PROGRAMS ON DISKETTES IF YOU HAVE A NORMAL IBM-PC OR AN IBM-PC-XT, SINCE THESE PC DO NOT HAVE 1.2 MEGABYTE DISK DRIVES).

PLOTTER ON WHICH PROGRAM PLOTTAB WILL OPERATE

THIS PROGRAM HAS A SIMPLE CALCOMP LIKE INTERFACE TO WHICHEVER PLOTTER IS USED. THE INTERFACE CONSISTS OF ONLY 3 SUBROUTINES...PLOTS, PLOT AND PEN. ALL CHARACTERS AND SYMBOLS ARE DRAWN USING SOFTWARE CONTROLLED TABLES CONTAINING X AND Y COORDINATES AND PEN POSITIONS WHICH ARE COMPLETELY PLOTTER INDEPENDENT. USING THESE CONVENTIONS THIS PROGRAM CAN BE INTERFACED TO USE ALMOST ANY PLOTTER OR GRAPHICS TERMINAL (SEE, PROGRAM PLOTTAB DOCUMENTATION FOR DETAILS).

FORMAT OF CODES AS DISTRIBUTED

THESE CODES REQUIRES A FORTRAN-77 COMPILER AND A SIMPLE CALCOMP LIKE GRAPHICS INTERFACE (FOR DETAILS SEE DOCUMENTATION OF PROGRAM PLOTTAB).

SUMMARY OF CONTENTS OF THE PLOTTAB TAPE

THIS CODE PACKAGE CONSISTS OF A MAGNETIC TAPE CONTAINING 15 FILES OF INFORMATION.

TAPE FILE	DESCRIPTION
1	PROGRAM LINTAB
2	LINTAB JOB CONTROL LANGUAGE AND INPUT PARAMETERS (BATCH DECK AND INPUT PARAMETERS TO EXECUTE PROGRAM)
3	LINTAB TABULATED CROSS SECTION OUTPUT HEATER TABULATED CROSS SECTION INPUT
4	LINTAB OUTPUT REPORT
5	PROGRAM HEATER
6	HEATER JOB CONTROL LANGUAGE AND INPUT PARAMETERS (BATCH DECK AND INPUT PARAMETERS TO EXECUTE PROGRAM)
7	HEATER TABULATED REACTION RATE OUTPUT
8	HEATER OUTPUT REPORT
9	PROGRAM PLOTTAB
10	SUBROUTINE PEN (DUMMY) (*)
11	SOFTWARE CHARACTER TABLE (*)
12	STANDARD SYMBOL AND LINE TYPE TABLE (*)
13	ALTERNATE SYMBOL AND LINE TYPE TABLE (*)
14	JOB CONTROL LANGUAGE AND INPUT PARAMETERS (BATCH DECK AND INPUT PARAMETERS TO EXECUTE PROGRAM)
15	OUTPUT REPORT

(*) FOR DETAILS SEE PROGRAM PLOTTAB DOCUMENTATION.

FILES 1 THROUGH 14 HAVE 80 CHARACTERS PER RECORD.
FILE 15 HAS 132 CHARACTERS PER RECORD.

IMPLEMENTING AND TESTING CODES

THE INPUT PARAMETERS SUPPLIED FOR THESE CODES ARE DESIGNED TO OPERATE ON THE INDICATED DATA AND TO PRODUCE THE OUTPUT REPORTS AND OUTPUT DATA INCLUDED ON THE TAPE (LINEAR AND HEATER) OR THE PLOTS (PLOTTAB) INCLUDED IN THE DOCUMENTATION FOR THESE PROGRAMS.

IN ORDER TO IMPLEMENT AND TEST THESE CODES IT IS SUGGESTED THAT THE USER,

(1) COMPILE AND LOAD THE PROGRAMS
(2) EXECUTE THE PROGRAMS USING THE INPUT PARAMETERS AND DATA SUPPLIED WITH THIS CODE PACKAGE.
(3) COMPARE THE RESULTS OBTAINED TO THE TEST RESULTS INCLUDED IN THIS CODE PACKAGE.

COMPILING AND CREATING LOAD MODULES ON IBM COMPUTERS

THE FOLLOWING JCL DECK ILLUSTRATES HOW TO COMPILE PLOTTAB AND CREATE A LOAD MODULE ON AN IBM COMPUTER. (1) A DUMMY SUBROUTINE PEN HAS BEEN CONCATENATED TO THE PROGRAM DURING COMPILATION TO PRODUCE BLACK-WHITE PLOTS (IGNOR ATTEMPTS TO CHANGE COLOR). (2) THE PROGRAM IS LINKED TO TO THE GRAPHICS SOFTWARE AVAILABLE AT IAEA TO PRODUCE PLOTS ON A BENSON-VARIAN PLOTTER (THIS PROCEDURE MAY DIFFER AT OTHER INSTALLATIONS).

EXAMPLE

```
//RNC1  JOB (NO,T),A2323-CULLEN,CLASS=I,MSGCLASS=X.NOTIFY=RNC,
//  TIME=(1,00)
//PASS1  EXEC  FORTCL,
//      LOADLIB='XNDC.EVALLIB',
//    DISP=SHR,
//      MEMBER=PLOTTAB
//FORT.SYSLIN DD SPACE=(800,(160,100))
//FORT.SYSIN  DD  DSN=XNDC.AANDM.SEND(PLOTTAB),DISP=SHR
//            DD  DSN=XNDC.AANDM.SEND(PEN),DISP=SHR
//LKED.SYSUT1  DD  SPACE=(1024,(800,300),RLSE)
//LKED.GR  DD  DSN=XCSX.VARIAN.LOAD,DISP=SHR
//LKED.SYSIN  DD  *
 INCLUDE GR(GRAPHICS)
//
```

REPORTING ERRORS

WE ARE ATTEMPTING TO MAKE THESE CODES AS COMPATIBLE AS POSSIBLE FOR USE WITH AS MANY DIFFERENT COMPUTERS AS POSSIBLE. IN ORDER TO HELP US AND TO INSURE THAT FUTURE VERSIONS OF THESE CODES AS COMPATIBLE AS POSSIBLE FOR USE AT YOUR INSTALLATION PLEASE REPORT ANY (REPEAT, ANY) COMPILER, LOADER OR EXECUTION DIAGNOSTICS OR PROBLEMS TO THE AUTHORS.

PLEASE REMEMBER IF YOU SIMPLY REPORT 'I'VE GOT A PROBLEM' AND DO NOT ADEQUATELY DESCRIBE EXACTLY HOW YOU WERE USING THE PROGRAMS IT WILL BE IMPOSSIBLE FOR THE AUTHORS TO HELP YOU. WHEN A PROBLEM ARISES PLEASE WRITE TO THE AUTHORS, DESCRIBE THE PROBLEM IN AS MUCH DETAIL AS POSSIBLE, IDENTIFY THE VERSION OF THE PROGRAM (E.G. VERSION 87-1) THAT YOU ARE USING AND SEND THE FOLLOWING INFORMATION ON MAGNETIC TAPE TO USING AND SEND THE FOLLOWING INFORMATION ON MAGNETIC TAPE TO THE AUTHOR,

(1) A COPY OF THE PROGRAM YOU ARE USING
(2) A COPY OF COMPILER DIAGNOSTICS (IF ANY)
(3) A COPY OF THE JCL DECK YOU USED TO EXECUTE THE PROGRAM
(4) A COPY OF THE OUTPUT REPORT FROM THE PROGRAM
(5) A COPY OF THE OUTPUT DATA (LINEAR OR HEATER)

IN ADDITION FOR PROGRAM PLOTTAB SEND,

(1) A COPY OF THE SOFTWARE CHARACTER TABLE
(2) A COPY OF THE SOFTWARE SYMBOL TABLE
(3) A COPY OF THE CURVE DATA
(4) A COPY OF THE DISCRETE POINT DATA
(5) A COPY OF THE PLOTS

WITHOUT ALL OF THIS INFORMATION IT IS IMPOSSIBLE TO EXACTLY SIMULATE THE PROBLEM THAT YOU RAN AND TO DETERMINE THE SOURCE OF YOUR PROBLEM.

CODE DOCUMENTATION

THESE CODES ARE DESIGNED TO BE SELF DOCUMENTING, IN THE SENSE THAT THE LATEST DOCUMENTATION FOR THE CODES INCLUDING A COMPLETE DESCRIPTION OF ALL INPUT PARAMETERS AND ASSIGNED INPUT/OUTPUT UNITS IS INCLUDED ON THE COMMENT CARDS AT THE BEGINNING OF THE CODES. PRINTED DOCUMENATION FOR THE CODES IS PERIODICALLY PUBLISHED. MOST OF THIS DOCUMENTATION CONSISTS OF A COPY OF THE COMMENT CARDS FROM THE BEGINNING OF THE CODES.
THE USER SHOULD BE AWARE THAT THE LATEST DOCUMENTATION IS ALWAYS THE THE COMMENT CARDS AT THE BEGINNING OF THE CODES (WHICH MAY SUPERSEDE THE MOST RECENT PRINTED DOCUMENTATION) AND THE USER SHOULD ALWAYS READ THE DOCUMENTATION IN THE CODES BEFORE USING THE CODES.

CONTENTS OF TAPE.

DISK FILENAMES DESCRIBED BELOW ONLY REFER TO THE CONVENTIONS USED AT THE NUCLEAR DATA SECTION, IAEA, VIENNA AND ARE ONLY INCLUDED BELOW FOR THE CONVENIENCE OF THE STAFF OF THE NUCLEAR DATA SECTION (I.E. THEY MAY BE IGNORED BY ALL OTHER PROGRAM USERS).

FILE	DESCRIPTION	RECORDS	RECORD LENGTH	DISK FILENAME XNDC.AANDM.SEND
1	PROGRAM LINTAB	1375	80	LINTAB
2	LINTAB JCL/INPUT PARAMETERS	58	80	GOLINTAB
3	LINTAB OUTPUT/HEATER INPUT	1270	80	LINOUT
4	LINTAB OUTPUT REPORT	1490	80	LINLIST
5	PROGRAM HEATER	1552	80	HEATER
6	HEATER JCL/INPUT PARAMETERS	32	80	GOHEATER
7	HEATER OUTPUT	1924	80	HEATOUT
8	HEATER OUTPUT REPORT	2123	80	HEATLIST
9	PROGRAM PLOTTAB	3863	80	PLOTTAB
10	SUBROUTINE PEN (DUMMY)	7	80	PEN
11	SOFTWARE CHARACTER TABLE	1468	80	CHARACTR
12	STANDARD SYMBOL/LINE TABLE	455	80	SYMBOLS1
13	ALTERNATE SYMBOL/LINE TABLE	516	80	SYMBOLS2
14	PLOTTAB JCL/INPUT PARAMETERS	24	80	GOPLOTTA

FILE	DESCRIPTION	RECORDS	RECORD LENGTH	DISK FILENAME XNDC.AANDM.REPORT
15	PLOTTAB OUTPUT REPORT	41	132	PLOTTAB
	TAPE TOTAL RECORDS	16198		