

MAINTENANCE AND VERSION IDENTIFICATION FOR NJOY

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Utilities for Maintenance

The maintenance methodologies of the CDC UPDATE utility program has been adopted for NJOY. It allows their users to keep track of the history of changes to the code and to document them. This utility exists with almost identical functions both in different makes of control data computers and of CRAY.

For other computers, similar utilities exist such as LIBRARIAN or HISTORIAN for IBM, which are to a large extent compatible with the UPDATE methodology. These software products are however available only on a commercial basis.

The UPDATE emulators have been developed in recent years in FORTRAN-77 and are therefore portable to a large extent to most computer makes. A more detailed description is annexed in the following.

These two utilities (UPEML-2.1 and UPDATE) are available from the code information centres such as the NEA Data Bank.

In order to facilitate users having access to different computers of taking advantage of the UPDATE procedure, only a subset of the update functions have been used for the NJOY maintenance. In fact, the non commercial UPDATE emulators do not reproduce the full capabilities of the CDC UPDATE.

Still, a few problems exist though in UPEML-2.1.

- Corrections of corrections (or overlapping corrections) cannot be carried out in the same update run. Overlap corrections must be carried out in separate steps in order to assure correct functioning
- Correction identifiers must start with an alphabetic character
- Recursive *COMDECK usage is not functioning.
(for additional restrictions, see report)

Description of UPEML and UPDATE

1. NAME OR DESIGNATION OF PROGRAM - UPEML.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED AND OTHER MACHINE VERSION PACKAGES AVAILABLE -

Program-name	Package-ID	Orig. Computer	Test Computer
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UPEML-2.1	PSR-0245/02	All Computers	All Computers

3. DESCRIPTION OF PROGRAM OR FUNCTION - UPEML is a machine-portable CDC UPDATE emulation program. It is capable of emulating a significant subset of the standard CDC UPDATE functions, including program library creation and subsequent modification.

4. METHOD OF SOLUTION - UPEML was written primarily to facilitate the use of CDC-based scientific packages on alternate computers such as the VAX 11/780, IBM 3081, Cray and others. Version 2.1 includes enhanced error checking, full ASCII character support, a program library audit capability, and a partial update option. Further enhancements include checks for overlapping corrections, processing of nested calls to common decks, and 'READ' and 'ADDFILE' directives to accommodate alternate input files and two quick update options.

6. TYPICAL RUNNING TIME - The time is dependent on the size of the source file.

PSR-0245/02: The test cases included in this program have been run at NEA-DB on both VAX-11/780 and IBM 3090/200 computers. Required CPU times did not exceed 3 seconds on IBM and 15 seconds on VAX for any of the cases.

9. STATUS -

PSR-0245/02 : Tested at NEADB May 1988

10. REFERENCES -

- "UPDATE, VERSION 1, Reference Manual," Revision 11/23/81, Report No. 60449900, Control Data Corporation.

PSR-0245/02 :

- T.A. Mehlhorn and M.F. Young:

UPEML Version 2.0: A Machine-Portable CDC Update Emulator. SAND87-0679, UC-32 (August 1987)

- T.A. Mehlhorn:

Release of UPEML Version 2.1 SANDIA NOTE (January 26, 1988)

- E. Sartori:

Note to All UPEML-2.1 Users NEADB Note NDB/88/0713 (May 9, 1988)

11. MACHINE REQUIREMENTS - UPEML is operable on a VAX, IBM, CDC and a CRAY computer.

PSR-0245/02: Main storage requirements for the test cases included in this package are: < 310K bytes on IBM 3090/200; 1400 peak page file size on VAX-11/780.

12. PROGRAMMING LANGUAGE USED.

PSR-0245/02 : FORTRAN-77

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED - A FORTRAN-77 compiler is required. The code was run at RSIC on the IBM 3033.

PSR-0245/02: VMS 4.4 (VAX-11/780); MVS (IBM 3090/200).

15. NAME AND ESTABLISHMENT OF AUTHORS -

Sandia National Laboratories

16. MATERIAL AVAILABLE -

PSR-0245/02 :

UPEML-2.1 Source with UPDATE Directives	4756 records
UPEML-2.1 General COMPILE File	4534 records
UPEML-2.1 JCL for IBM MVS Computers	244 records
UPEML-2.1 Source for IBM Compiler (80char/1)	4543 records
UPEML-2.1 COMPILE file for IBM (87char/1)	4543 records
UPEML-2.1 JCL for Interactive Use on VAX	150 records
UPEML-2.1 JCL for Batch Submission on VAX	51 records
UPEML-2.1 COMPILE File for VAX (87char/1)	4543 records
UPEML-2.1 ABORT subroutine for VAX	3 records
UPEML-2.1 COMPILE File for CRAY (87char/1)	4568 records
UPEML-2.1 S.P. 1 create new program library	19 records
UPEML-2.1 S.P. 1 LISTFL print from IBM & VAX	29 records
UPEML-2.1 S.P. 1 print out from IBM	42 records
UPEML-2.1 S.P. 1 print out from VAX	41 records
UPEML-2.1 S.P. 2 LISTFL print from IBM	11 records
UPEML-2.1 S.P. 2 print out from IBM	49 records
UPEML-2.1 S.P. 2 print out from VAX	48 records
Source file produced by S.P. 2 (IBM & VAX)	15 records
UPEML-2.1 S.P. 3 (correct + compile file)	17 records
UPEML-2.1 S.P. 3 print out from IBM	50 records
UPEML-2.1 S.P. 3 print out from VAX	48 records
UPEML-2.1 S.P. 3 LISTFL print from IBM	25 records
Source file produced by S.P. 3 (IBM & VAX)	24 records

1. NAME OR DESIGNATION OF PROGRAM - UPDATE.

2. COMPUTER FOR WHICH PROGRAM IS DESIGNED AND OTHER MACHINE VERSION
PACKAGES AVAILABLE -

Program-name	Package-ID	Orig. Computer	Test Computer
UPDATE	PSR-0270/01	IBM	3033

3. DESCRIPTION OF PROGRAM OR FUNCTION - UPDATE is a FORTRAN source file manipulator which allows the editing of source files without entering an editor program. It runs interactively on Data General MV computers and may be adapted to run on an IBM interactive system.

4. METHOD OF SOLUTION - UPDATE initially builds a program library from a input source deck. The source input is a FORTRAN code with UPDATE directives embedded in the file. Once a program library is created, a compilable source file may be extracted from it using the proper UPDATE directive. Changes to the program library are also possible by making what are called correction runs.

6. TYPICAL RUNNING TIME - Both sample input cases took less than a second of CPU time on the IBM 3033.

9. STATUS -

PSR-0270/01 : Arrived at NEADB June 1989

10. REFERENCES -

PSR-0270/01 :
- B.L. Kirk:
UPDATE - A Fortran-77 Source File Manipulator.
NUREG/CR-4478, ORNL/TDMC-4 (January 1989)

11. MACHINE REQUIREMENTS - The code runs on the Data General MV family of computers and the IBM 3033 or 3081.

12. PROGRAMMING LANGUAGE USED.

PSR-0270/01 : FORTRAN-77

13. OPERATING SYSTEM UNDER WHICH PROGRAM IS EXECUTED - A FORTRAN 77 compiler is required. The Data General version runs under AOS/VS, and the IBM version runs under MVS or MVS-XA.

15. NAME AND ESTABLISHMENT OF AUTHORS -

Contributed by: Radiation Shielding Information Center
Oak Ridge National Laboratory
Oak Ridge, Tennessee, U. S. A.

16. MATERIAL AVAILABLE -

PSR-0270/01 :
JCL, Sample Problem 1 (input to NEWP.CLI),
Sample Problem 2 (input to CORRECT.CLI),
UPDATE Source Program (Fortran-77),
Output compilation from S.P. 1, Output compilation from S.P. 2,
report NUREG/CR-4478, ORNL/TDMC-4 (January 1989).

Version Identification

Starting from NJOY-89 every correction set is identified by the letters Unnn where $1 < nnn < 999$. This version number is also updated together with the date of update in the NJOY banner produced at the beginning of the output listing.

This enables users to trace back which exact version they have used for producing cross-section libraries and identify with better precision the effects of specific modifications to NJOY. An example of this procedure is shown in the following:

```
*/ updates for njoy89
*/ the naming convention is njoy 89.nnn
*/ where nnn is the number of the last ident in this file
*/ except for "vers", which contains the value of nnn and the date.
*/ -----
*ident up1
*/ groupr -- 25 may 89 -- add elements to separation energy calculation
*i groupr.4609
   if (iza.eq.74000) iza=74184
*ident up2
*/ acer -- 25 may 89 -- add elements to separation energy calculation
*i acer.5957
   if (iza.eq.74000) iza=74184
*ident up3
*/ heatr -- 25 may 89 -- add elements to separation energy calculation
*i heatr.2398
   if (iza.eq.74000) iza=74184
   if (iza.eq.74000) iza=74184
*ident up4
*/ acer -- 30 may 89 -- set thermal pendf unit number
*i acer.6003
   nin=npend
*ident up5
*/ plotr -- 1 jun 89 -- misc. fixes
*d plotr.66
c   *           60 characters allowed.           *
*d plotr.71
c   *           60 characters allowed.           *
*d plotr.76,80
c   *           1 = linear x - linear y           *
c   *           2 = linear x - log y              *
c   *           3 = log x - linear y             *
c   *           4 = log x - log y                *
c   *           set negative for 3d axes          *
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*d plotr.110
c * 60 characters allowed. *
*d plotr.130
c * 60 characters allowed. *
*d plotr.142
c * 60 characters allowed. *
*i plotr.163
c * ntp not used *
c * nkh not used *
*d plotr.222
c * 60 characters allowed. *
*i plotr.228
c * (.le.0 to omit vector) *
*d plotr.234
c * defaults=5.,2.,2. *
*d plotr.1184
96 format(/41h ***error in plotr***error in axis input.)
*i plotr.1618
c (.le.0 to omit vector)
*i plotr.1628
if (xpoint.le.0.) go to 130
*d plotr.1640
130 xtp=xposn(xtag,ytag)
*i plotr.1642
if (xpoint.le.0.) return
*d plotr.1771
*i plotr.1775
c
*/ -----
*ident up6
*/ thermr -- 4 jun 89 -- better eprime grid for calcem
*d thermr.1373
nbeta=2
*d thermr.1376,1377
isab=ibeta+nbeta
a(ibeta)=0.
a(ibeta+1)=25.
----- etc -----

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