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**PROSDOR –
An IBM-3090 Based
Semi-Automated Procedure
Linking HERMES MCNP and
KORIGEN for the Burnup
Analysis of Accelerator
Driven Cores**

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Accelerator Driven Cores

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PROSDOR -

AN IBM-3090 BASED SEMI-AUTOMATED PROCEDURE LINKING HERMES MCNP AND KORIGEN FOR THE BURNUP ANALYSIS OF ACCELERATOR DRIVEN CORES.

ABSTRACT

This report guides the user of PROSDOR in the execution of the various calculational steps needed to carry out a burnup study of a fission subcritical target driven by high energy protons. The introduction of the files and programs involved is made in close reference to the procedural chronological execution steps. The PROSDOR is a dedicated linkage between the HERMES, MCNP, and KORIGEN codes. At this point it is limited to a cylindrical homogenous target, enabling the analysis of a truly homogenous core or a hard spectrum lattice, with planned upgrading.

PROSDOR-

EINE IBM-3090 BASIERTE HALBAUTOMATISCHE PROZEDUR ZUR VERKNÜPFUNG VON HERMES, MCNP UND KORIGEN FÜR DIE ABBRANDANALYSE BESCHLEUNIGER GETRIEBENER CORES.

ZUSAMMENFASSUNG

Dieser Bericht ist eine Anleitung für den Benutzer von PROSDOR bei der Durchführung der verschiedenen Rechenschritte zur Erstellung einer Abbrandstudie für ein durch hochenergetische Protonen getriebenes unterkritisches Spalttarget. Die benötigten Datensätze (Files) und Programme werden entsprechend dem zeitlichen Ablauf der einzelnen Rechenschritte eingeführt. PROSDOR ist eine Verknüpfung der Codes HERMES, MCNP und KORIGEN. Die Anwendungsmöglichkeit von PROSDOR ist zur Zeit auf ein zylindrisches homogenes Target beschränkt; dabei sind sowohl Analysen von streng homogenen Cores als auch von Gittern mit einem harten Spektrum möglich. Weiterentwicklung ist geplant.

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1.0 SCOPE

PROSDOR is an IBM-3090 based semi-automated linkage between the codes HERMES /1/ , MCNP3 /2/ , KORIGEN /3/ , developed to enable a consistent and complete analysis of the burnup of proton driven subcritical cores. The analysis includes, among other, the time dependent core criticality and power and the evolution of nuclei transmutations.

Presently PROSDOR is limited to homogenous cylindrical cores, commonly also 'targets', injected at base with high energy protons. Allowed, none theless, are lattice structures, provided the neutron energy spectrum is hard enough to render the lattice fuel pitch much smaller than the neutron mean free path. In fact PROSDOR was put together in the first place to conduct a study of transmutations in Na cooled lattices.

Left for a future upgrade is the automation of burnup calculations for heterogeneous layouts, namely sectioned cores and thermal lattices. This will entail not merely an automated transfer of larger data bodies, but also modifications and re-definitions of notions to have HERMES-MCNP derived output comply with KORIGEN practices.

The target mixture may contain up to 20 - 25 nuclei. It is determined by a limit of 90 MCNP tally requests, as explained in the next section.

As concerns the application of HERMES, any element of the KfK NUKLIDKARTE /4/ (some 2500 ground and meta-stable states), may be in the target, either directly loaded or produced by spallations, fissions, captures, $(n,2n)$, $(n,3n)$, and decay. This large scope of allowable nuclei is the result of rebasing the KORIGEN libraries on all the NUKLIDKARTE data and by extending the HERMES capacity to mass numbers beyond 239.

The application of MCNP is limited, however, by the availability of MCNP formatted cross sections. At this point the availability list extends to 120 elements, including actinides, structural materials, moderators, and fission products of generally known interest.

The methodology served by PROSDOR is detailed in ' A METHODOLOGY FOR THE NEUTRONIC ANALYSIS OF FISSION CORES DRIVEN BY ACCELERATED PROTONS', by M. Segev, submitted for publication in Nucl. Sci. Eng.

2.0 THE 'PROSDOR' PROCEDURE - STEP BY STEP

TABLE 1. PROCEDURE FLOW TABLE FOR 'PROSDOR'

all files mentioned, excluding those in the "load modules" column, are card image files.

STEP	LOAD MODULES REQUIRED	SUBMIT (EXEC) FILES	INPUT FILES, NEEDED FOR THE SUBMITTAL	OUTPUT FILES, LATER IN USE AS 'SUBMIT'S OR INPUTS	OUTPUT FILES, SOME FOR INTERNAL PROSDOR USE
////////////////////////////////////					
1	B.O.C. CORE DEFINE	B2HM +	B2HM.INP + HM.OLD.L + HM.OLD.S +	HM.L HM.S	
2	B.O.C. CORE CALC.	HERSEG.LOAD MCNP3A.LOAD	HM.L KOR.ACLIB + KOR.FPLIB + KOR.RUN0 + SPLDCY.HD + YIELDLIB +	KORLIB.AC KORLIB.FP KORRUN TRG.PRNTOUT	SUBMIT.FILE HERMES.OUTPUT NTRN.SORC SPLL.PRDCTS SPLDCY.KINP MCNP.OUTPUT YIELD.LIST
3	B.O.C. AND SUBSEQ. CORE CALC.	HERSEG.LOAD MCNP3A.LOAD	HM.S KOR.RUN0 + SPLDCY.HD + YIELDLIB +	KORRUN TRG.PRNTOUT	SUBMIT.FILE HERMES.OUTPUT NTRN.SORC SPLL.PRDCTS SPLDCY.KINP MCNP.OUTPUT
4	BURNUP OF N DAYS	KORSEG.LOAD	KORRUN(N) KORLIB.AC KORLIB.FP KORLIB.SR +	KOROUT	
5	REPLACE CORE NUCLEI DENSITIES	K2HM +	KOROUT TRG.PRNTOUT HM.S	HM.S.NEW	
6	RENAME 'HM.S.NEW' 'HM.S' AND RETURN TO STEP 3				

+ files that should be available prior to step 1.

<<<<< **STEP 1** >>>>>

B2HM is the file to execute ('exec' file) in order to generate two files with BOC data for the execution of BOC HERMES/MCNP. Input files required for executing B2HM are two 'old' HERMES/MCNP exec files, namely HM.OLD.L and HM.OLD.S (the meaning of the characterizations 'L' and 'S' will be given shortly), assumed available (hence 'OLD'), plus a 'user-organized' data file by the name B2HM.INP. The content and structure of this latter file is next exemplified.

TABLE 2. EXAMPLE OF THE BOC INPUT FILE 'B2HM.INP'

```

-----
////////////////////////////////////
20 TARGET ELEMENTS (1ST LINE OF 'B2HM.INP')
ELEMENT IDENTIFICATIONS, DENSITIES AND TALLIES
      Z  A    MCNP3      DENSITY      N2N N3N <----FISSIONS----> N,C
      016 017 018 019 020 021 038 102
-----
  1  6   12   6012.10C  G  0.1240E+00  /+ /+ / / / / / / / / / / /+
  2  8   16   8016.04C  G  0.2900E-02  /+ /+ / / / / / / / / / / /+
  3 11   23  11023.01C  G  0.1040E-02  /+ /+ / / / / / / / / / / /+
  4 26   56  26000.11C  G  0.4230E-02  /+ /+ / / / / / / / / / / /+
  5 43   99  43099.00C  G  0.1111E-06  /+ /+ / / / / / / / / / / /+
  6 44  100  44100.00C  G  0.7214E-03  /+ /+ / / / / / / / / / / /+
  7 44  101  44101.00C  G  0.1111E-06  /+ /+ / / / / / / / / / / /+
  8 53  129  53129.00C  G  0.3140E-02  /+ /+ / / / / / / / / / / /+
  9 54  129  54129.00C  G  0.3943E-03  /+ /+ / / / / / / / / / / /+
 10 54  130  54130.00C  G  0.7493E-04  /+ /+ / / / / / / / / / / /+
 11 94  238  94238.00C  G  0.1418E-04  /+ /+ /+ / / / / / / / / /+
 12 94  239  94239.00C  G  0.4398E-03  /+ /+ / / /+ /+ /+ / / /+
 13 94  240  94240.00C  G  0.2562E-03  /+ /+ /+ / / / / / / / / /+
 14 94  241  94241.00C  G  0.9910E-04  /+ /+ /+ / / / / / / / / /+
 15 94  242  94242.00C  G  0.5445E-04  /+ /+ /+ / / / / / / / / /+
 16 95  241  95241.00C  G  0.1111E-06  /+ /+ /+ / / / / / / / / /+
 17 95  242  95242.01C  M  0.1111E-06  /+ /+ /+ / / / / / / / / /+
 18 95  243  95243.00C  G  0.1111E-06  /+ /+ /+ / / / / / / / / /+
 19 96  244  96244.00C  G  0.1111E-06  /+ /+ /+ / / / / / / / / /+
 20 96  245  96245.00C  G  0.1111E-06  /+ / / / / /+ /+ / / / / /+

////////
/73.00/ TARGET RADIUS (CM)
/146.0/ TARGET HEIGHT (CM)
/1600./ PROTONS ENERGY (MEV)
/102.0/ PROTON CURRENT (MILIAMPS)
/3.000/ ENERGY PER FISSION (WATTS*SEC/10**11)
/ 20/ NO. OF BATCHES IN HERMES (EACH BATCH 100 PROTONS)
/ 9000/ MAX NO. OF MCNP SOURCE NEUTRONS
/ 6.0/ MAX TIME (MINUTES) IN MCNP.SHORT
/ 6.0/ MAX TIME (MINUTES) IN MCNP.LONG

```

```

//////// (MCNP RUN TERMINATES WHEN EITHER THE TIME LIMIT
        OR THE NO.OF SOURCE NEUTRONS LIMIT IS REACHED)
////////////////////////////////////

```

'B2HM.INP' EXPLAINED

```

line 1: no. of elements in the target mixture (N) (I2)
line 2: heading
line 3: heading
line 4: heading
line 5: heading
line 6: 1st elmnt ,14 data (2(I2,2X),I3,2X,A9,2X,A1,1X,E11.4,8(3X,A1))
line 7: 2nd elmnt ,14 data (2(I2,2X),I3,2X,A9,2X,A1,1X,E11.4,8(3X,A1))
lines 8,9,10...each 14 data (2(I2,2X),I3,2X,A9,2X,A1,1X,E11.4,8(3X,A1))
line N+5, Nth elmnt,14 data (2(I2,2X),I3,2X,A9,2X,A1,1X,E11.4,8(3X,A1))

```

on each of the last N lines the 14 data carry the following meaning:

- data item 1: element no. in the list.
- data item 2: atomic number of element (Z).
- data item 3: mass number of element (A).
- data item 4: MCNP name for the xsection table of the element
- data item 5: 'G' or 'M', denoting ground or meta-stable state.
- data item 6: element density in units of 10**24 atoms/cc.
- data item 7: '+' if the MCNP xsection table includes (n,2n).
- data item 8: '+' if the MCNP xsection table includes (n,3n).
- data item 9: '+' if the MCNP xsection table includes fission as "18".
- data item 10: '+' if the MCNP xsection table includes fission as "19".
- data item 11: '+' if the MCNP xsection table includes fission as "20".
- data item 12: '+' if the MCNP xsection table includes fission as "21".
- data item 13: '+' if the MCNP xsection table includes fission as "38".
- data item 14: '+' if the MCNP xsection table includes (n,gamma).

If (Z,A), read as a single number (e.g. Z=94 A=239, read as 94239), identifies an element, then the elements must come in an increasing order of their identifiers. The meta-stable and ground states of an element, when both entered, must come in this order. Element 54129 must be on the list (with density zero), for the approximate treatment of fission product poisoning in PROSDOR. The number of '+' entries must not exceed 90.

line N+6 (namely the line next to the last element data line): empty

```

line N+ 7: heading
line N+ 8: target radius, cm (1X,A5)
line N+ 9: target height, cm (1X,A5)
line N+10: protons energy, MeV (1X,A5)
line N+11: protons current, mA (1X,A5)
line N+12: energy per fission (watts*sec/10**11) (1X,A5)
line N+13: no.of batches in HERMES, 100 protons per batch (1X,A5)
line N+14: max no. of source neutrons to be run in MCNP (1X,A5)
line N+15: time limit (min.) for the HM.S run (1X,A5)
line N+16: time limit (min.) for the HM.L run (1X,A5)

```

All last 9 entries should be right adjusted.

User handling of target data is confined to 'B2HM.INP', with a single exception: the burnup period (in days) will have to be entered into the KORIGEN exec file, as later explained.

The execution of B2HM will generate two files, namely HM.L and HM.S, discussed next in the description of STEP 2 and STEP 3.

The issue of MCNP xsection tables is taken up in a special section below. The user may find out for himself or herself which of the eight possible reactions actually exist in a given MCNP xsection table by executing MCNP (or HM.L, for that matter) and consulting the MCNP output (file MCNP.OUTPUT). Knowing in advance which tallies *not* to request is necessary in order to maximize the number of elements which define the target mix. The execution of HM.L is the subject of the next subsection.

<<<<< **STEP 2** >>>>>

HM.L is mnemonic for HERMES-MCNP-LONG. It is a procedure to execute in sequence HERMES, then MCNP; it contains interspaced programming pieces which properly link between HERMES and MCNP, as between the HERMES-MCNP results and subsequent KORIGEN executions. The characterization 'LONG' has to do with MCNP input request tallies, by which effective 1-group microscopic cross sections are generated so that the KORIGEN data bases may be appropriately updated. In a target specified as a mixture of some 20 elements there are about 90 tallies involved, augmenting the run time of MCNP per source neutron to almost an order of magnitude more than for the same target without these tallies request. The update of KORIGEN data bases will be discussed later; at this point suffice it to say that practice enables one to conduct a burnup study, with little loss of accuracy, if the HM execution files for time steps subsequent to BOC are defined without these tallies request, namely by giving up KORIGEN data base updates. The HM exec files which lack these tallies request are named HM.S, S for 'SHORT', meaning (relatively) short-time neutron histories in the target.

Two load modules are involved in the execution of HM.L, namely HERSEG.LOAD and MCNP3A.LOAD. The first is compiled from an adaptation of the KFA HERMES code. In this adaptation the HERMES was upgraded to deal with mass numbers greater than 239, and with more than 10 elements per target mix, and some of its results were redefined and reorganized to suit the purpose of PROSDOR. The second is a compilation of the original MCNP3A.

Five permanent files exist, which serve as input files for executing HM.L. KOR.ACLIB and KOR.FPLIB are mnemonics for KORIGEN ACTINIDES LIBRARY and KORIGEN FISSION PRODUCTS LIBRARY. In these two libraries the decay data encompass some 2500 ground and meta-stable states, covering the KfK NUKLIDKARTE entries from Hydrogene to Einsteinium. In the PROSDOR termi-

nology every element of these 2500, is both an 'actinide' and a 'fission product' as the application may be. Both KOR.ACLIB and KOR.FPLIB contain these decay data; KOR.ACLIB contains also 1G xsections, for fission, capture, (n,2n), and (n,3n), for some 'typical' fast spectrum. These two 'libraries' serve as bases for the update to be performed during the HM.L execution. YIELDLIB is a file containing the f.p yield lists for fissions of 12 specific nuclei; the single 'target-integrated' yield, as required in PROSDOR terminology, is generated based on these 12 lists. KOR.RUN0 is a file for a KORIGEN execution and, as with the KOR.ACLIB and KOR.FPLIB, its purpose is to serve as a basis into which proper KORIGEN run items will be inserted during the HM.L execution. SPLDCY.HD is a 'head' for a KORIGEN exec file, its purpose is to serve as a head to a list of the spallation products, organized as relative densities for a KORIGEN run for the effect of a decay field without a neutron flux.

The HM.L execution produces four files of intimate relation to the PROSDOR procedure. KORLIB.AC is a KORIGEN library, containing 1G cross sections for the (20 or so) elements defining the target mix, proper for the target spectrum at hand. KORLIB.FP is a KORIGEN library containing the single 'target-unified' yield list for all spallations and fissions, as actually take place in the target (many hundreds of nuclei involved). KORRUN is an exec file for a burnup step with KORIGEN, designed to calculate the density changes in the target elements based on the actual target flux, and on actual 1G xsections and nuclei yields, as reflected in the KORLIB.AC and KORLIB.FP. TRG.PRNTOUT is a file containing a selection of HM input and output, relating to the performance of the target at BOC, and of possible interest to the user. A TRG.PRNTOUT from an HM.L run is next exemplified.

EXAMPLE OF 'TRG.PRNTOUT' FOR AN 'HM.L' RUN

////////////////////////////////////

target input

target radius (cm) = 73.0
target height (cm) = 146.0
target volume (m**3) = 2.4443
proton current (miliamps) = 102.0
protons energy (mev) = 1600.0
watts per fission (*10**11) = 3.00

extractions from the hermes run

element	number density	gr/cc in target	total tons in target
1 60120	0.1240e+00	2.47073	6.03912
2 80160	0.2900e-02	0.07704	0.18832
3 110230	0.1040e-02	0.03972	0.09708
4 260560	0.4230e-02	0.39333	0.96139
5 430990	0.1111e-06	0.00002	0.00004

6	441000	0.7214e-03	0.11978	0.29278
7	441010	0.1111e-06	0.00002	0.00005
8	531290	0.3140e-02	0.67258	1.64396
9	541290	0.3943e-03	0.08446	0.20644
10	541300	0.7493e-04	0.01617	0.03953
11	942380	0.1773e-04	0.00701	0.01713
12	942390	0.5498e-03	0.21819	0.53330
13	942400	0.3203e-03	0.12764	0.31199
14	942410	0.1239e-03	0.04958	0.12119
15	942420	0.6806e-04	0.02735	0.06685
16	952410	0.1111e-06	0.00004	0.00011
17	952420	0.1111e-06	0.00004	0.00011
18	952430	0.1111e-06	0.00004	0.00011
19	962440	0.1111e-06	0.00005	0.00011
20	962450	0.1111e-06	0.00005	0.00011

(fisrah) fissions per proton = 0.308
 (yiop) total nuclei yield per proton = 7.270
 (trop) transmutation events per proton = 8.751
 (fherm) total flux (cm) per proton = 0.1286e+03

microscopic transmutation cross sections

1	60120	0.4060
2	80160	0.4870
3	110230	0.6160
4	260560	1.1060
5	430990	1.6040
6	441000	1.6140
7	441010	1.6250
8	531290	1.8980
9	541290	1.8980
10	541300	1.9070
11	942380	2.7440
12	942390	2.7510
13	942400	2.7570
14	942410	2.7640
15	942420	2.7700
16	952410	2.7640
17	952420	2.7700
18	952430	2.7770
19	962440	2.7830
20	962450	2.7890

(enop) neutrons below 20 mev per proton = 16.68 (+- 1.3 percent)

statistics : 2000 histories in 127.43 seconds

extractions from the mcnp run

number-density sum is .137440

density fractions are

1	6012.10c	0.9012e+00	g
2	8016.04c	0.2111e-01	g

3	11023.01c	0.7560e-02	g
4	26000.11c	0.3079e-01	g
5	43099.00c	0.1111e-05	g
6	44100.00c	0.5240e-02	g
7	44101.00c	0.1111e-05	g
8	53129.00c	0.2284e-01	g
9	54129.00c	0.2870e-02	g
10	54130.00c	0.5400e-03	g
11	94238.00c	0.1300e-03	g
12	94239.00c	0.4000e-02	g
13	94240.00c	0.2330e-02	g
14	94241.00c	0.9000e-03	g
15	94242.00c	0.4900e-03	g
16	95241.00c	0.1111e-05	g
17	95242.01c	0.1111e-05	m
18	95243.00c	0.1111e-05	g
19	96244.00c	0.1111e-05	g
20	96245.00c	0.1111e-05	g

multiplication is 17.17

(fisram) fission rate per neutron = 0.8454e+01
 (capram) capture rate per neutron = 0.1487e+02
 (xnnram) n,xn rate per neutron = 0.0000e+00
 (percik) percent neutron leakage = 5.97
 (avenue) no. of neutrons per fission = 2.91
 (estimk) estimated (lg) criticality = 0.993

target power = 2698.5 mw

target power density = 1.104 mw/liter

beam power = 163.2 mw

k-effective of target = 0.945

10**	-9	-	-8	mev	-----	spectfrac = 0.00000
10**	-8	-	-7	mev	-----	spectfrac = 0.00000
10**	-7	-	-6	mev	-----	spectfrac = 0.00008
10**	-6	-	-5	mev	-----	spectfrac = 0.00783
10**	-5	-	-4	mev	-----	spectfrac = 0.04279
10**	-4	-	-3	mev	-----	spectfrac = 0.12147
10**	-3	-	-2	mev	-----	spectfrac = 0.18148
10**	-2	-	-1	mev	-----	spectfrac = 0.23118
10**	-1	-	0	mev	-----	spectfrac = 0.27494
10**	0	-	1	mev	-----	spectfrac = 0.13993
10**	1	-	2	mev	-----	spectfrac = 0.00031
10**	2	-	3	mev	-----	spectfrac = 0.00000
10**	3	-	4	mev	-----	spectfrac = 0.00000
10**	4	-	5	mev	-----	spectfrac = 0.00000
10**	5	-	6	mev	-----	spectfrac = 0.00000
10**	6	-	7	mev	-----	spectfrac = 0.00000

(fmcnp) total flux (cm) per neutron = 0.2286e+04 (+- 47.3 percent)

flux-spectrum averaged neutron energy = 0.036 mev

for a proton beam of 102.0 miliamps target flux = 0.996e+16 n/s/cm2

elemental rates per neutron

	capture	fission	n,2n	n,3n
60120	0.2921e-02	0.0000e+00	0.0000e+00	0.0000e+00
80160	0.4196e-05	0.0000e+00	0.0000e+00	0.0000e+00
110230	0.1754e-01	0.0000e+00	0.2786e-04	0.0000e+00

260560	0.2172e+00	0.0000e+00	0.1352e-02	0.0000e+00
430990	0.8361e-03	0.0000e+00	0.1586e-06	0.0000e+00
441000	0.6106e+00	0.0000e+00	0.0000e+00	0.0000e+00
441010	0.7421e-03	0.0000e+00	0.4083e-06	0.8619e-09
531290	0.5126e+01	0.0000e+00	0.4223e-02	0.5254e-04
541290	0.2031e+01	0.0000e+00	0.1833e-02	0.6580e-05
541300	0.4421e-01	0.0000e+00	0.1061e-03	0.2072e-05
942380	0.1197e+00	0.6791e-01	0.5038e-05	0.8699e-06
942390	0.3603e+01	0.6020e+01	0.6797e-03	0.3514e-05
942400	0.2713e+01	0.3398e+00	0.4816e-03	0.4300e-04
942410	0.6125e+00	0.2412e+01	0.9425e-03	0.1943e-04
942420	0.4582e+00	0.4763e-01	0.1675e-03	0.1675e-04
952410	0.1967e-02	0.9257e-04	0.8289e-07	0.2322e-08
952421	0.3823e-03	0.2710e-02	0.4536e-06	0.2549e-07
952430	0.2364e-02	0.6720e-04	0.2095e-06	0.1128e-07
962440	0.1438e-02	0.1468e-03	0.1841e-06	0.5257e-08
962450	0.3949e-03	0.2261e-02	0.1859e-06	0.0000e+00

statistics : 15 histories in 6.06 minutes

target summary highlights

total single yield (hermes + mcnp fission) = 1.921

1 group effective cross sections

60120	f,c,2n,3n	mic.x-sections	-	1.36e-03	1.03e-05	0.00e+00	0.00e+00
80160	f,c,2n,3n	mic.x-sections	-	1.64e-03	6.31e-07	0.00e+00	0.00e+00
110230	f,c,2n,3n	mic.x-sections	-	2.07e-03	7.35e-03	1.17e-05	0.00e+00
260560	f,c,2n,3n	mic.x-sections	-	3.72e-03	2.24e-02	1.39e-04	0.00e+00
430990	f,c,2n,3n	mic.x-sections	-	5.39e-03	3.28e+00	6.23e-04	0.00e+00
441000	f,c,2n,3n	mic.x-sections	-	5.43e-03	3.69e-01	0.00e+00	0.00e+00
441010	f,c,2n,3n	mic.x-sections	-	5.46e-03	2.91e+00	1.60e-03	3.38e-06
531290	f,c,2n,3n	mic.x-sections	-	6.38e-03	7.12e-01	5.86e-04	7.30e-06
541290	f,c,2n,3n	mic.x-sections	-	6.38e-03	2.25e+00	2.03e-03	7.28e-06
541300	f,c,2n,3n	mic.x-sections	-	6.41e-03	2.57e-01	6.18e-04	1.21e-05
942380	f,c,2n,3n	mic.x-sections	-	1.68e+00	2.94e+00	1.24e-04	2.14e-05
942390	f,c,2n,3n	mic.x-sections	-	4.78e+00	2.86e+00	5.39e-04	2.79e-06
942400	f,c,2n,3n	mic.x-sections	-	4.72e-01	3.69e+00	6.56e-04	5.85e-05
942410	f,c,2n,3n	mic.x-sections	-	8.50e+00	2.16e+00	3.32e-03	6.84e-05
942420	f,c,2n,3n	mic.x-sections	-	3.14e-01	2.94e+00	1.07e-03	1.07e-04
952410	f,c,2n,3n	mic.x-sections	-	3.73e-01	7.72e+00	3.25e-04	9.11e-06
952421	f,c,2n,3n	mic.x-sections	-	1.06e+01	1.50e+00	1.78e-03	1.00e-04
952430	f,c,2n,3n	mic.x-sections	-	2.73e-01	9.28e+00	8.22e-04	4.43e-05
962440	f,c,2n,3n	mic.x-sections	-	5.86e-01	5.64e+00	7.23e-04	2.06e-05
962450	f,c,2n,3n	mic.x-sections	-	8.88e+00	1.55e+00	7.30e-04	0.00e+00

for a proton beam of 102.0 miliamps target flux = 0.996e+16 n/s/cm2
 eff. (hrms-trm + mcnp-f/c/2n/3n) trnsn.xsection = 0.079 barns
 target power = 2698.5 mw
 target power density = 1.104 mw/liter
 beam power = 163.2 mw
 k-effective of target = 0.945

korigen fission products library updated
and given the name "prsd.korlib.fp"

korigen actinides library updated
and given the name "prsd.korlib.ac"
(eff.xsections of target elements updated in the actinides library)

//

The execution of HM.L generates also some other files. SUBMIT.FILE is a HERMES-original, containing a list of nuclei and neutron events, as extracted from the original HETC 'history tape'. HERMES.OUTPUT is the (almost) original HERMES output, containing integral and distributed quantities above 20 MeV of neutron energy. NTRN.SORC is a list, compiled from SUBMIT.FILE, of phase space neutron coordinates, in format appropriate for source to the MCNP program. SPLD.PRDCTS is a detailed list of the number of times spallations produced each (Z,A) element. SPLDCY.KINP is a KORIGEN exec file, organizing the said list into a KORIGEN input, so that a decay without neutron flux can be performed on the yields of the list. MCNP.OUTPUT is the original MCNP output, with input and output detail, statistics and integral quantities of interest. YIELD.LIST is a user transparent list of the relative , 'spallation + fission integrated' nuclei yields in the target. Most of these output files are used internally in the PROSDOR procedure. They are not destroyed, so that the user may access them for possible checks, or for other benefits.

<<<<< **STEP 3** >>>>>

HM.S is mnemonic for HERMES-MCNP-SHORT. 'S' is used to distinguish it from HM.L, namely to characterize it as a HERMES-MCNP execution file without tallies request for the generation of effective 1G microscopic xsections for an update of the 'actinides' KORIGEN library. Likewise, the 'fission-product' KORIGEN library is not updated in executing HM.S.

Input files for the execution of HM.S are KOR.RUN0, SPLDCY.HD, and YIELDLIB. The functions of these files was explained above, in the subsection 'STEP 2', in conjunction with the execution of HM.L.

The output files generated in the HM.S execution are a subset of the set of output files generated in the HM.L execution. Again, reference to subsection 'STEP 2' above will clarify the functions of these files.

HM.S, being considerably faster than HM.L, should provide, within a reasonable run time, a good estimate of target entities such as the flux and the power. The user must be aware, though, that the closer is the target to criticality the longer it takes for MCNP to follow through the history of a source neutron, hence the

smaller is the number of histories processed within the user-specified run time limit.

<<<<< **STEP 4** >>>>>

The execution of a burnup step is performed with KORRUN. It is an exec file, generated in the preceding step (step 3) and ready for submittal, except that the user must specify in it the time duration, in days, of the burnup interval. The flux value for the burnup calculation is the flux of the target, as previously calculated with HM.S (step 3 above) and already existing in KORRUN as a datum. The 'AC' and 'FP' libraries for the run have been properly generated in step 2 above. An example of a KORRUN file is next given

TABLE 3. EXAMPLE OF 'KORRUN'

```

-----
////////////////////////////////////
//INROV0KG JOB (00V0,101,P6P4D),SEGEV,NOTIFY=INROV0,MSGCLASS=H,
// REGION=3072K,TIME=(3,00)
//*FORMAT PR,DDNAME=,DEST=PINR1
//*MAIN LINES=20
//*
//* SUBMIT-DATEI : *****
//*
//* K O R I G E N FOR DECAY OF SPALLATION PRODUCTS
//*
// EXEC TSO
  ERASE PRSD.KOROUT
/*
// EXEC F7G,NAME=KORIGEN
//STEPLIB DD DSN=INROV0.KORSEG.LOAD,DISP=SHR,LABEL=(,,IN)
//G.FT03F001 DD SYSOUT=*,DCB=*.FT06F001
//G.FT30F001 DD UNIT=INR,DISP=(NEW,CATLG),SPACE=(TRK,(5,5)),
// DCB=(BLKSIZE=3520,RECFM=FB,LRECL=133),DSN=INROV0.PRSD.KOROUT
//G.FT09F001 DD SYSOUT=*,DCB=*.FT06F001
//G.FT45F001 DD SYSOUT=*,DCB=*.FT06F001
//G.FT07F001 DD DSN=INROV0.PRSD.KORLIB.SR,DISP=SHR,LABEL=(,,IN)
//G.FT07F002 DD DSN=INROV0.PRSD.KORLIB.AC,DISP=SHR,LABEL=(,,IN)
//G.FT07F003 DD DSN=INROV0.PRSD.KORLIB.FP,DISP=SHR,LABEL=(,,IN)
//G.SYSIN DD *
NUCLEAR DATA LIBRARY
  20
  60120  80160 110230 260560 430990 441000 441010 531290 541290
541300 942380 942390 942400 942410 942420 952410 952420 952430
962440 962450
  1.      1.      1.      1.00E-25      0 0 0 0
  3      3      0      1      0      3      -1      0      0      7      0      0      0
                                0
                                11      1
                                11      1

```

```

0
1
IRRADIATION
1.85+15 1.11+00 1.11+00
99.00 100.00 101.00
TEST NUCLIDES
86400.0 D
1.000E-10 1.000E-10 1.200E-10 1.000E-03 1.000E-03 1.000E+06 1.000E+06 1.000E-03
60120.1240E+00 80160.2900E-02 110230.1040E-02 260560.4226E-02 430990.1016E-06 2
441000.7144E-03 441010.6503E-05 531290.3081E-02 541290.5656E-03 541300.1531E-03 2
942380.1259E-04 942390.3565E-03 942400.2601E-03 942410.9480E-04 942420.5496E-04 2
952410.1221E-05 952420.9419E-07 952430.4414E-05 952440.6718E-06 952450.1206E-06 2

0 0
//
////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////

```

The number of days for the required burnup is to be input by the user, replacing the '99.00' entry, two lines below 'IRRADIATION'. The entry immediately above it is the flux (neutrons per sec per cm^2). The example includes two extra irradiation periods (with negligible flux levels), the purpose of this inclusion is to guide the user as to the format in which extra irradiation periods (total of 9) are to be input, should the user wish to take advantage of the KORRUN file in setting up a series of burnup steps. As an example to such use is the possibility of repeating all the burnup steps of a given cycle in one KORRUN execution, once the flux level for each of the burnup periods has been determined previously by a PROSDOR procedure (namely a series of HERMS-MCNP-KORIGEN linked executions).

The load module for the execution of KORRUN is KORSEG.LOAD. It is compiled from a special adaptation of KORIGEN to suit terminology and requirements in PROSDOR, in particular the requirement that any of the elements appearing in the KfK NUKLIDKARTE be an 'actinide' or a 'fission product' as the application may be, and the requirement that all fission and spallation products be presented in a single unified yield list, target and burnup step dependent. This is unlike the 'classical' KORIGEN practice of having 12 different f.p distributions, each the yield of the fission of one of (certain) 12 fissionable elements.

The KORRUN file contains, in proper format, the target nuclei densities at the beginning of the burnup period. The KORLIB.AC and KORLIB.FP, needed as inputs for the execution of KORRUN, have been generated in the preceding step 2. KORLIB.SR is a dummy-input structural materials file.

The output file in this step is KOROUT, essentially the KORIGEN usual output file. In it the user may find end-of-period densities organized under the headings of both 'actinides' and 'fission products'. Under the first heading come all the target mix elements, as all are declared 'actinides' in KORRUN. Changes in densities under this heading are due to the target elements undergoing spallations and fissions in the HERMES regime, as well as fissions, (n,gamma), (n,2n), and (n,3n) in the MCNP regime. Under the second heading comes an extensive list of

element densities. All entries in the 'charge' ('beginning-of-period') column are zero, as none of the target mix nuclei is defined as f.p. in KORRUN. The end-of-period densities reflect a combined production rate by all reactions in the HERMES regime and fissions in the MCNP regime.

<<<<< STEP 5 >>>>>

K2HM is mnemonics for 'KORIGEN to HERMES-MCNP'. The function of this exec file is to update HM.S with the new target densities, as calculated in KOROUT in the preceding step. In addition this program interprets the KOROUT given accumulated total f.p density from the preceding burnup as an added density to element 54129, namely to the element whose poisoning effect is chosen as a close representation of the true total poisoning effect of the fission products.

Input files to the execution of K2HM are KOROUT (generated in step 4), TRG.PRNTOUT (generated in step 3) and HM.S (the exec file for step 3).

The output file is HM.S.NEW; should the cycle continue, this file is to be re-named HM.S and step 3 re-initiated.

3.0 MCNP CROSS SECTION TABLES

The JCL cards for the execution of MCNP3, shown below, identify 7 binary files which contain the current body of recommended MCNP3 cross section tables, namely:

```
INR0V0.MCNP3A.PELLOAT2
INR0V0.MCNP3A.PELLOFP2
INR0V0.MCNP3A.PELLOMX2
INR0V0.MCNP3A.PELLOMM2
INR0V0.MCNP3A.PELLOMM2
INR0V0.MCNP3A.PELLOMM2
INR415.MCNP3A.BMCCS2
INR415.MCNP3A.EFF1CH2
```

Table 5, following the JCL extract, lists 120 elements, showing for each an MCNP3 name and a file (out of the 7 above) in which resides the cross section table for that name. Depending on the origin of the binary cross section table, an element may have a few names with corresponding different residence files. There are also instances of different names in one and the same file, reflecting different evaluated data bodies.

**TABLE 4. AN EXTRACT OF MCNP JCL CARDS
MENTIONING THE BINARY XSECTION FILES FOR MCNP3**

```
////////////////////////////////////
//L.LOAD DD DISP=SHR,DSN=INR415.MCNP3A.LOAD
//L.SYSIN DD *
  INCLUDE LOAD(MCNP3A)
  ENTRY MCNP
//G.XSDIR DD DISP=SHR,DSN=INR0V0.MCNP3A.XSDIR2,LABEL=(,,IN)
//G.EFF1CH2 DD DISP=SHR,DSN=INR415.MCNP3A.EFF1CH2,LABEL=(,,IN)
//G.BMCCS2 DD DSN=INR415.MCNP3A.BMCCS2,DISP=SHR,LABEL=(,,IN)
//G.PELLOAC2 DD DSN=INR0V0.MCNP3A.PELLOAT2,DISP=SHR,LABEL=(,,IN)
//G.PELLOFP2 DD DSN=INR0V0.MCNP3A.PELLOFP2,DISP=SHR,LABEL=(,,IN)
//G.PELLOMX2 DD DSN=INR0V0.MCNP3A.PELLOMX2,DISP=SHR,LABEL=(,,IN)
//G.PELLOMM2 DD DSN=INR0V0.MCNP3A.PELLOMM2,DISP=SHR,LABEL=(,,IN)
//G.PELLOMM2 DD DSN=INR0V0.MCNP3A.PELLOMM2,DISP=SHR,LABEL=(,,IN)
//G.PELLOMM2 DD DSN=INR0V0.MCNP3A.PELLOMM2,DISP=SHR,LABEL=(,,IN)
//G.PELLOMM2 DD DSN=INR0V0.MCNP3A.PELLOMM2,DISP=SHR,LABEL=(,,IN)
//G.INPUT DD *
//G.OUTPUT DD SYSOUT=*,DCB=*.FT06F001
//G.OUTP DD DSN=INR0V0.PRSD.MCNP.OUTPUT,UNIT=INR,SPACE=(TRK,(10,10)),
// DCB=(LRECL=133,BLKSIZE=3857,RECFM=FBA),DISP=(NEW,CATLG)
//G.RUNTPE DD DSN=INR0V0.MCNP.TEST.SOURCE,UNIT=INR,
// SPACE=(TRK,(10,10)),DCB=(RECFM=VBS,LRECL=X,BLKSIZE=8184),
// DISP=(NEW,CATLG)
```

```

//G.FT39F001 DD DSN=&&TEMP1,UNIT=SYSDA,DISP=(NEW,PASS),
// DCB=(RECFM=FB,LRECL=133,BLKSIZE=5320),
// SPACE=(TRK,(10,5))
//G.FT40F001 DD DSN=&&TEMP2,UNIT=SYSDA,DISP=(NEW,PASS),
// DCB=(RECFM=FB,LRECL=133,BLKSIZE=5320),
// SPACE=(TRK,(10,5))
//G.FT08F001 DD DSN=INR0V0.PRSD.NTRN.SORC,DISP=SHR
//G.INP      DD *
MESSAGE:XSDIR=XSDIR

```

////////////////////////////////////

TABLE 5. RECOMMENDED MCNP3 CROSS SECTION TABLES FOR 'PROSDOR'

ORIGIN:	-- ENDF-B/IV --	----- JEF2 -----	---- EFF1 -----			
	NAME OF ELEMENT	NAME OF BINARY FILE	NAME OF ELEMENT	NAME OF BINARY FILE	NAME OF ELEMENT	NAME OF BINARY FILE
H	1	1001.04C	BMCCS2		1001.91C	EFF1CH2
H	2	1002.02C	BMCCS2		1002.91C	EFF1CH2
H	3	1003.03C	BMCCS2		1003.91C	EFF1CH2
HE	NAT	2000.01C	BMCCS2			
HE	3	2003.03C	BMCCS2		2003.91C	EFF1CH2
HE	4	2004.03C	BMCCS2		2004.91C	EFF1CH2
LI	6	3006.10C	BMCCS2		3006.91C	EFF1CH2
LI	7	3007.05C	BMCCS2		3007.91C	EFF1CH2
BE	9	4009.03C	BMCCS2		4009.91C	EFF1CH2
B	NAT	5000.01C	BMCCS2			
B	10	5010.03C	BMCCS2		5010.91C	EFF1CH2
B	11	5011.02C	BMCCS2		5011.91C	EFF1CH2
C	NAT				6000.91C	EFF1CH2
C	12	6012.10C	BMCCS2			
N	14	7014.04C	BMCCS2		7014.91C	EFF1CH2
O	16	8016.04C	BMCCS2		8016.91C	EFF1CH2
F	19	9019.03C	BMCCS2		9019.91C	EFF1CH2
NA	23	11023.01C	BMCCS2		11023.91C	EFF1CH2
MG	NAT	12000.02C	BMCCS2		12000.91C	EFF1CH2
AL	27	13027.04C	BMCCS2		13027.91C	EFF1CH2
SI	NAT	14000.02C	BMCCS2		14000.91C	EFF1CH2
P	31	15031.01C	BMCCS2		15031.91C	EFF1CH2
S	32	16032.01C	BMCCS2		16032.91C	EFF1CH2
CL	NAT	17000.02C	BMCCS2		17000.91C	EFF1CH2
AR	NAT	18000.01C	BMCCS2			
AR	40				18040.91C	EFF1CH2

TABLE 5 (CONTINUED)

ORIGIN:	-- ENDF-B/IV --	----- JEF2 -----	---- EFF1 -----
	NAME OF ELEMENT	NAME OF BINARY FILE	NAME OF ELEMENT
		NAME OF ELEMENT	NAME OF BINARY FILE
K NAT	19000.01C	BMCCS2	19000.91C EFF1CH2
CA NAT	20000.10C	BMCCS2	20000.91C EFF1CH2
TI NAT	22000.11C	BMCCS2	22000.91C EFF1CH2
V NAT	23000.30C	BMCCS2	23000.91C EFF1CH2
CR NAT	24000.11C	BMCCS2	24000.91C EFF1CH2
MN 55	25055.01C	BMCCS2	25055.91C EFF1CH2
FE NAT	26000.11C	BMCCS2	26000.91C EFF1CH2
CO 59			27059.91C EFF1CH2
NI NAT	28000.11C	BMCCS2	28000.91C EFF1CH2
NI 58	28058.01C	BMCCS2	
CU NAT	29000.10C	BMCCS2	29000.91C EFF1CH2
ZN 64		30064.00C	PELLORM2
GA NAT	31000.01C	BMCCS2	
SR 90		38090.00C	PELLOFP2
ZR NAT	40000.02C	BMCCS2	40000.91C EFF1CH2
ZR 90		40090.00C	PELLOFP2
ZR 91		40091.00C	PELLOFP2
ZR 92		40092.00C	PELLOFP2
ZR 93		40093.00C	PELLOFP2
NB 93	41093.30C	BMCCS2	41093.91C EFF1CH2
MO NAT	42000.01C	BMCCS2	42000.91C EFF1CH2
TC 99		43099.00C	PELLOFP2
RU 99		44099.00C	PELLOFP2
RU 100		44100.00C	PELLOFP2
RU 101		44101.00C	PELLOFP2
RU 102		44102.00C	PELLOFP2
AG 107			47107.91C EFF1CH2
AG 109			47109.91C EFF1CH2
CD NAT	48000.01C	BMCCS2	48000.91C EFF1CH2
IN 113			49113.91C EFF1CH2
IN 115			49115.91C EFF1CH2
SN NAT	50000.01C	BMCCS2	
SN NAT	50999.02C	BMCCS2	
SN 114			50114.91C EFF1CH2
SN 115			50115.91C EFF1CH2
SN 116			50116.91C EFF1CH2
SN 117			50117.91C EFF1CH2
SN 118			50118.91C EFF1CH2
SN 119			50119.91C EFF1CH2
SN 120			50120.91C EFF1CH2
SN 122			50122.91C EFF1CH2
SN 124			50124.91C EFF1CH2
I 127		53127.00C	PELLOFP2

TABLE 5 (CONTINUED)

ORIGIN:	-- ENDF-B/IV --	----- JEF2 -----	----- EFF1 -----	
	NAME OF ELEMENT	NAME OF BINARY FILE	NAME OF ELEMENT	NAME OF BINARY FILE
I 129		53129.00C PELLOFP2		
XE 128		54128.00C PELLOFP2		
XE 129		54129.00C PELLOFP2		
XE 130		54130.00C PELL0MX2		
CS 133			55133.91C EFF1CH2	
CS 137		55137.00C PELL0MX2		
BA 134			56134.91C EFF1CH2	
BA 135			56135.91C EFF1CH2	
BA 136			56136.91C EFF1CH2	
BA 137		56137.00C PELL0MX2	56137.91C EFF1CH2	
BA 138	56138.01C BMCCS2	56138.00C PELL0MX2	56138.91C EFF1CH2	
LA 139		57139.00C PELL0MX2		
EU NAT	63000.01C BMCCS2			
GD NAT	64000.01C BMCCS2			
HO 165	67165.01C BMCCS2			
HF NAT			72000.91C EFF1CH2	
TA 181	73181.02C BMCCS2		73181.91C EFF1CH2	
W NAT	74000.01C BMCCS2			
W 182	74182.10C BMCCS2		74182.91C EFF1CH2	
W 183	74183.10C BMCCS2		74183.91C EFF1CH2	
W 184	74184.10C BMCCS2		74184.91C EFF1CH2	
W 186	74186.10C BMCCS2		74186.91C EFF1CH2	
PT NAT	78000.01C BMCCS2			
AU 197	79197.10C BMCCS2			
PB NAT	82000.10C BMCCS2		82000.91C EFF1CH2	
PB NAT	82000.99C BMCCS2			
BI 209			83209.91C EFF1CH2	
TH 232	90232.10C BMCCS2			
PA 233		91233.00C PELLOAC2		
U 233	92233.10C BMCCS2			
U 234	92234.10C BMCCS2			
U 235	92235.11C BMCCS2	92235.00C PELL0MM2		
U 236	92236.01C BMCCS2	92236.00C PELL0MX2		
U 237	92237.01C BMCCS2	92237.00C PELL0MX2		
U 238	92238.12C BMCCS2	92238.00C PELL0MM2		
U 239	92239.01C BMCCS2			
U 240	92240.01C BMCCS2			
NP 237		93237.00C PELL0MX2		
NP 238		93238.00C PELL0MX2		
NP 239		93239.00C PELL0MX2		
PU 238	94238.01C BMCCS2	94238.00C PELL0MX2		
PU 239	94239.17C BMCCS2	94239.00C PELL0MM2		
PU 240	94240.12C BMCCS2	94240.00C PELL0RM2		

TABLE 5 (CONTINUED)

ORIGIN:	-- ENDF-B/IV --		----- JEF2 -----		---- EFF1 -----	
	NAME OF ELEMENT	NAME OF BINARY FILE	NAME OF ELEMENT	NAME OF BINARY FILE	NAME OF ELEMENT	NAME OF BINARY FILE
PU 241	94241.01C	BMCCS2	94241.00C	PELLORM2		
PU 242			94242.00C	PELLOAT2		
PU 243	94243.31C	BMCCS2	94243.00C	PELLOAT2		
AM 241			95241.00C	PELLOAT2		
AM 242			95242.00C	PELLOAT2		
AM 242M	95242.01C	BMCCS2	95242.11C	PELLOAT2		
AM 243			95243.00C	PELLOAT2		
CM 242			96242.00C	PELLOAT2		
CM 243			96243.00C	PELLOAT2		
CM 244			96244.00C	PELLOAT2		
CM 245			96245.00C	PELLOAT2		

For ENDF, JEF, EFF and for the definition of reaction types see /5/ , /6/ , /7/ .

4.0 PROSDOR, SIMPLY, FOR THE HURRIED USER

one: make sure the following load modules are available:

HERSEG.LOAD
MCNP3A.LOAD
KORSEG.LOAD

two: make sure the following card image files are available before starting at B.O.C.

B2HM
HM.OLD.L
HM.OLD.S
KOR.ACLIB
KOR.FPLIB
KOR.RUN0
SPLDCY.HD
YIELDLIB
KORLIB.SR
K2HM

three: start- at BOC: organize your (only) input file
B2HM.INP
(see- section 2. 'step 1' above)

four: submit- B2HM
obtain- HM.L
HM.S

five: submit- HM.L
obtain- KORLIB.AC
KORLIB.FP
KORRUN
TRG.PRNTOUT

six: submit- HM.S
obtain- KORRUN
TRG.PRNTOUT

seven: insert- N, number of days for the burnup step in KORRUN
(see- section 2. 'step 4' above)
submit- KORRUN(N)
obtain- KOROUT

eight: submit- K2HM
obtain- HM.S.NEW
rename- HM.S.NEW → HM.S
return- to step 'six' above

5.0 RUN TIME CONSIDERATIONS.

The input file B2HM.INP includes an entry for the no. of proton batches for the HERMES execution. Each batch contains 100 protons. The user has to find out by experience the average run time per batch. This time is an increasing function of the target size and average nuclei mass number. The former is due to decreased leakage; the latter is due to an increase in the run time spent per particle, as there are more high energy fissions per higher mass nucleus. HERMES will come to a normal halt, namely with the usual output, whichever of the following two limits occurs first: the requested no. of protons, or the HM job card time limit.

The execution stop for MCNP is given both by a maximum on the no. of source neutrons to be followed and a time limit. MCNP will come to a normal halt, provided one of these limits is satisfied within the HM job card time allocation. If a certain percentage of the HM job time request is spent in HERMES, the MCNP will have available only the remainder time; if, by the consumption of this remainder, neither of the two MCNP proper stop limits is satisfied MCNP will come to an abnormal stop, without its regular output: the PROSDOR will thus abnormally end.

MCNP will not come to a normal end if the target is super critical; the MCNP run will then end with a message 'BANK IS FULL'. This type of abnormal end will frequently occur also with criticalities in the range between .97 and 1, as there may be certain neutron histories with a very long chain of fission events prior to neutron escape, overburdening the code.

There are no special time considerations for KORRUN (KORIGEN run); as a rule a KORRUN execution will always end within 3 minutes of a job card time specification. The execution of B2HM and K2HM is almost immediate.

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