

3.1 Control Function

3.1.1 Control Data

Summary	This unit defines miscellaneous control data including the duration of the calculation and the type of processing.
Use	This unit must always be included in a complete, executable MCBEND calculation.
Methods	<p>The Monte Carlo processing ends when a time limit is reached, when a given number of samples have been taken, or when a specified standard deviation has been reached. These parameters may be supplied as input data.</p> <p>The random sampling of the Monte Carlo method uses calls to an internal random number generator. A facility is provided to set the initial seeds for the random number generator as an aid to achieving reproducible results. The random number generator can also be moved forward through the sequence (nudged) from a given initial setting. This can be used to bypass part of the sequence or to reproduce particle histories without repeating a complete calculation.</p> <p>For long, complex calculations it is usual to execute a series of MCBEND calculations via a Dump/Restart facility. Requests for a dump are made in this unit.</p>

Relationship with other units.

Dataset Definitions	The SOURCE ONLY option requires a source log file to be assigned in the Dataset Definitions Unit. The DUMP INTERVALS option requires dump files to be assigned in the Dataset Definitions Unit. The use of a designated SOURCE PART with a source file assigned in the Dataset Definitions Unit means that the particle positions and directions (in the source file) are transformed to the local co-ordinate frame of the part.
Material Geometry	The use of a designated SOURCE PART is affected by the Fractal Geometry model. If the part is referenced by name then the name must correspond to that used in the part definition.
Material Specification	The use of material names in the SOURCE MATERIALS lists must be consistent with the names assigned in the material definitions.
Simple Source Geometry & Complex Source	The use of a designated SOURCE PART affects the co-ordinate system used for defining source geometries.
Tabular Output	The REPORT INTERIM RESULTS and STOP AT SDLIMIT OF options require the results to be specified in the Tabular Output Unit.

Notes on Sheet 1

- 1 **READ** = Read and check each input unit independently. Generate a Library Input if **LIBRARY CREATE** keywords were supplied before Control Data Unit.

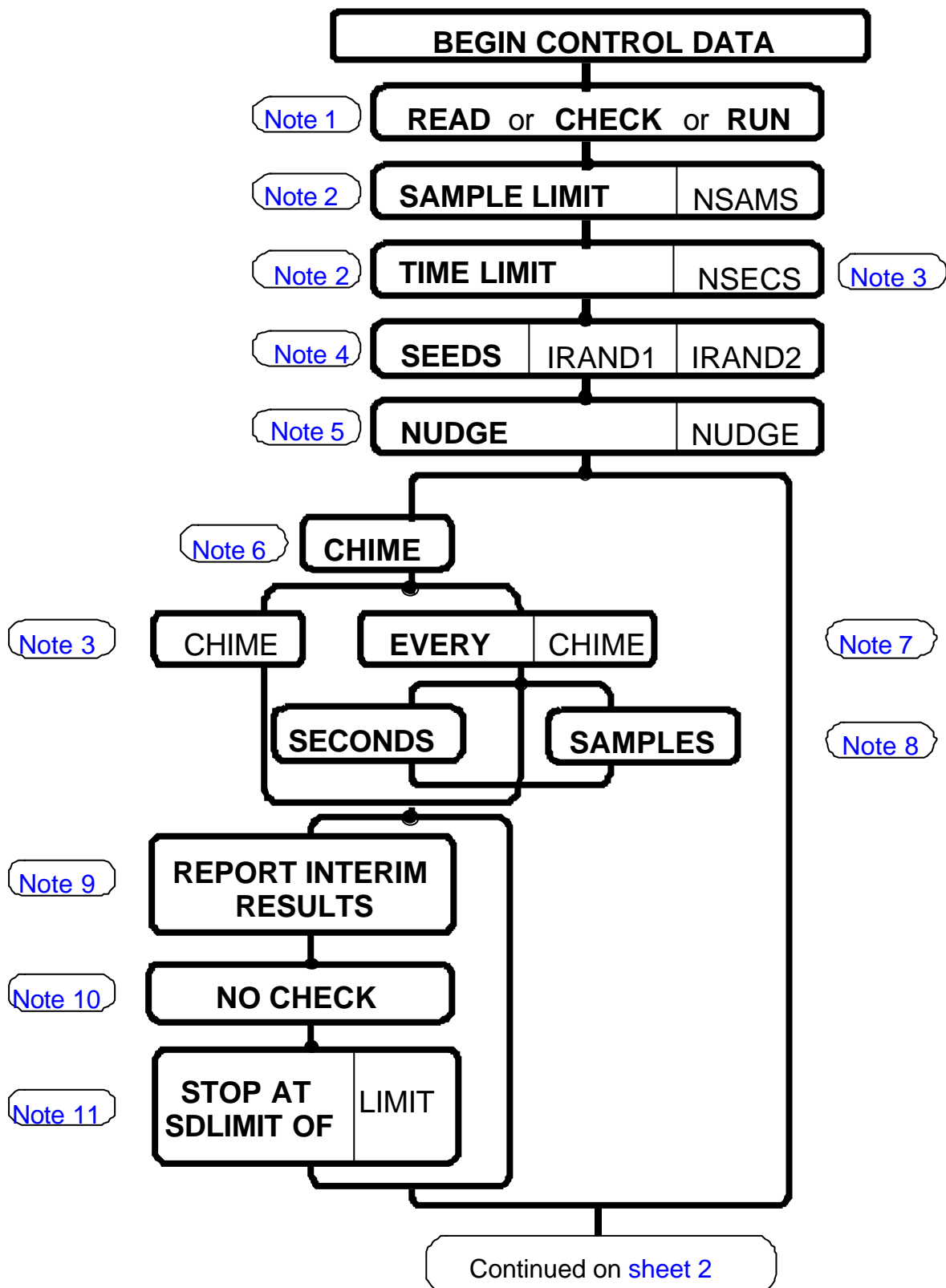
 CHECK = As **READ** + Check units for consistency and completeness. Evaluate importance map, process nuclear data and set up calculation ready for sampling to begin.
- RUN** = As **CHECK** + Execution of Monte Carlo calculation. (Sampling begins) This is the default.
- 2 The length of the calculation may be controlled by specifying the number of the last sample to be taken or by defining the C.P.U time to be used for sampling. If both limits are set then execution stops at the first limit reached. If neither is set then the calculation is controlled by the resources allocated to the job. This facility may not be available on every type of machine. The default sample limit is 2,147,483,647 and the default time limit is 10,000,000. Note that under Windows 9x the specified time limit is the *elapsed* time.
- 3 Values of time may be real or integer and optionally be followed by the keyword **S** (seconds) **M** (minutes) or **H** (hours) to provide more convenient units. The code converts to integer seconds before storing and printing.
- 4 Initial seed values (>0) for the random number generator. Default values are derived from the date and time.
- 5 This option moves the random number generator to a point corresponding to **NUDGE** calls having been made since initial seeding.
- 6 This option generates a simple output message every **CHIME** intervals to indicate the progress of the job during sampling.
- 7 This option allows the chime interval to be defined in a more detailed manner than by just inputting a time.
- 8 This option selects that the **CHIME** is performed on a sample basis rather than on a time basis. The default is **SECONDS**.
- 9 This option allows the current results to be printed after each **CHIME**. The results to be printed are selected via the Tabular Output Unit. After the second batch of results are printed the code performs checks on the validity of the results. The checks are described in Chapter 6 Advice and Examples, Section 6.2.7.
- 10 This option turns off the code checks on the validity of the results. **INTERIM RESULTS** are still produced.
- 11 This allows the run to be terminated when a specified Standard Deviation is reached. The tables defined in the Tabular Output Unit are used to specify which data are to be used to determine when the run is to be stopped. **LIMIT** is the percentage Standard Deviation (where **LIMIT** is a real number).

Back Compatibility

The following keywords from earlier versions of MCBEND are not included in the flow charts but are recognised by the code.

RANDOM NUMBER GENERATORS, PROCESS TO STAGE ONE / TWO / THREE, SPLITTING/NO SPLITTING.

Sheet 1: Control Data

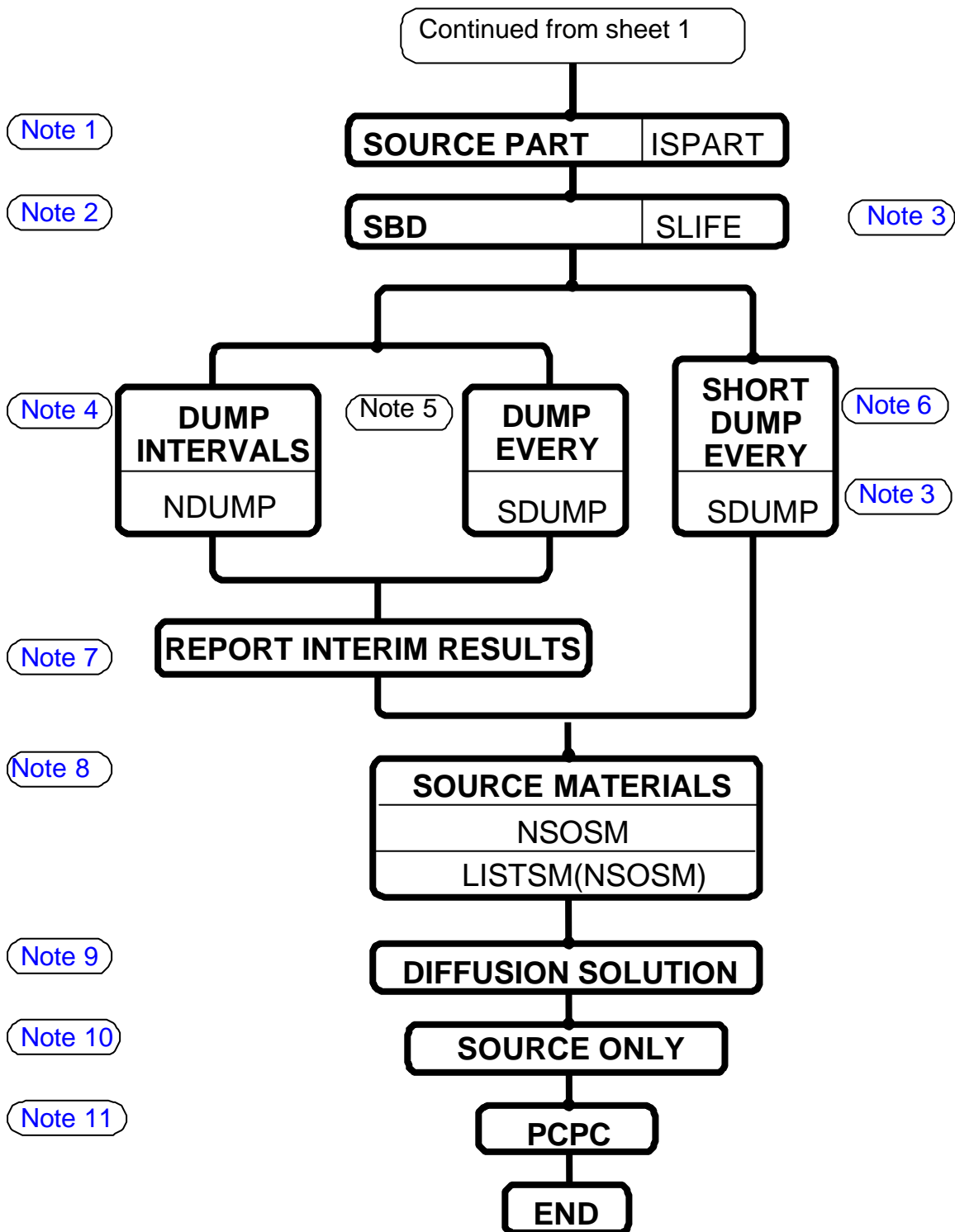


Notes on Sheet 2

- 1 If the Simple or Complex Source modules are being used, the distribution of sources in the problem *may be defined* using the local co-ordinate system of a particular part in the Fractal Geometry model. If, in a secondary calculation, a First Flight Source is being used then the particle positions and directions from a source file *may be transformed* to the local co-ordinate frame of a particular part.

An FG part (only one) may be identified here as the one that holds the source definition. When source co-ordinates have been sampled they are transformed to the global co-ordinate frame using the rotation matrix and translation vector of the source part. If the source part appears in several locations in the assembled model then a source point will be assigned to a randomly selected occurrence of the part. If the simple source is used with automatic weighting in conjunction with the source part option the calculation will be inefficient. The referenced part may optionally be an alphanumeric name corresponding to a named part in Material Geometry Unit.
- 2 This option avoids futile histories by placing a limit on the time spent tracking any single sample. Up to ten particles may be terminated by reaching their 'sell by date' before execution is stopped.
- 3 Values of time may be real or integer and optionally be followed by the keyword **S** (seconds) **M** (minutes) or **H** (hours) to provide more convenient units. The code converts to integer seconds before storing and printing.
- 4 This option defines the number of dumps to be taken during the calculation. A value of 1 requests a dump at the end of job completion; a value of 0 (or non-use of the option) signifies that no dump is required.
- 5 This alternative to the above option requests a dump to be taken every SDUMP seconds (or minutes or hours, see Note 3).
- 6 A short dump is restricted to results and data defining the problem. It is not suitable for restarts but provides shorter, quicker dumps for post-MCBEND processing packages. A short dump is written to an unformatted file assigned by the user to the named channel SDUMP in the DATSETS file.
- 7 This option allows the current results to be printed after each dump. The results to be printed are selected via the Tabular Output Unit. After the second batch of results are printed the code performs checks on the validity of the results. The checks are described in Chapter 6 Advice and Examples, Section 6.2.7.
- 8 The source may optionally be restricted to zones containing a material declared in the list LISTSM. NSOSM defines the number in the list. Source points sampled in other zones are rejected and appropriate normalisation factors applied. The materials referenced in the list may include alphanumeric names.
- 9 This option requests an approximate, scoping calculation to be carried out using a diffusion theory solution instead of Monte Carlo. It is restricted to neutron calculations with a simple, separable source. By default, the diffusion solution uses method E cross-sections from the MEDCON 33 group neutron library. A 28 group method D calculation may be selected by appending the keyword **D**. For explanation of the group schemes see Chapter 4 Input Appendices, Appendix D, Tables D2.1 and D2.4.
- 10 This option (principally for diagnostic purposes) limits the code activity to the sampling of source points without tracking.
- 11 This option causes MCBEND to emulate the well logging diffusion code PC².

Sheet 2: Control Data



Examples

- 1 BEGIN CONTROL DATA
RUN
TIME LIMIT 7200 or TIME LIMIT 120M or TIME LIMIT 2H
END

- 2 BEGIN CONTROL DATA
RUN
DUMP INTERVALS 1
END

- 3 BEGIN CONTROL DATA ! A MCBEND7 example.
PROCESS TO STAGE THREE
SAMPLE LIMIT 1000
TIME LIMIT 30
DUMP INTERVALS 2
RANDOM NUMBER GENERATORS 123 957
SPLITTING
END

- 4 BEGIN CONTROL DATA ! Above example In MCBEND10
SAMPLE LIMIT 1000
TIME LIMIT 30
DUMP INTERVALS 2
SEEDS 123 957
END

- 5 BEGIN CONTROL DATA
RUN
SAMPLE LIMIT 5000
SBD 20M ! Chop any sample taking > 20 min.
CHIME 1H ! Write a message every hour.
DUMP INTERVALS 5 ! Take a dump every 1000 samples.
REPORT INTERIM RESULTS ! Produce interim results each dump
SEEDS 123 456 ! Set random number seeds.
NUDGE 1000 ! Simulate 1000 calls to the random
END ! number generator since seeds.

- 4 This example splits a run of 60000 samples into 6 equal batches for which interim results are produced and checked.

BEGIN CONTROL DATA
SAMPLE LIMIT 60000
CHIME EVERY 10000 SAMPLES
REPORT INTERIM RESULTS
SOURCE PART capsule ! The source is defined in the local
! geometry of the FG part named 'capsule'
SOURCE MATERIALS 3 ! Sources are restricted to 3 specified materials
1 8 Steel ! 'Steel' is refers to a material defined with this
! name in the Material Specification Unit

END

3.1.2 Dataset Definitions

Summary This unit identifies the output channels associated with various files which may optionally be written by MCBEND.

Use This unit may be omitted if none of the options is required.

Methods A number of FORTRAN input/output channels are referenced and allocated for specific input/output operations. Many files, including those identified here, now have fixed channel numbers and are referenced in the DATSETS file by **name**. Others have channels (>30) assigned by the user, and these are referenced in the DATSETS file by **number** (see Chapter 2 Input Description). Dataset Definitions Unit is still required since it is used to request MCBEND to open that type of file.

The following options are available: dump files, which contain all the information about the current state of execution of the code; processed nuclear data files, for use in subsequent cases using the same materials; source particle log files, to facilitate the analysis of source behaviour (or to be used in a subsequent MCBEND run as a source file); collision files, for coupling point energy neutron/gamma cases or to provide sources for other codes (e.g. RANKERN); and leakage particle parameter files, to facilitate the analysis of escaping particles or to link calculations.

Relationship with other units

Control Data If **DUMPA/B** is requested then the number of dump intervals is stated in Control Data Unit.

Output Control The events recorded on a **COLLISION FILE** may be restricted to particular types by data supplied in Output Control Unit.

Energy Data & Material Specification If the type of calculation is a point-energy neutron case (Energy Data Unit) then the processed nuclear data for the materials specified in the Material Specification Unit may be saved for use in a similar problem. If such data has already been created by this mechanism, and is being retrieved, then the Material Specification Unit must be omitted from the input.

Energy Data A channel must be allocated to a **SOURCE FILE** if this is the form of source sampling requested in the Energy Data Unit (i.e. COLLISION SOURCE or FIRST FLIGHT SOURCE).

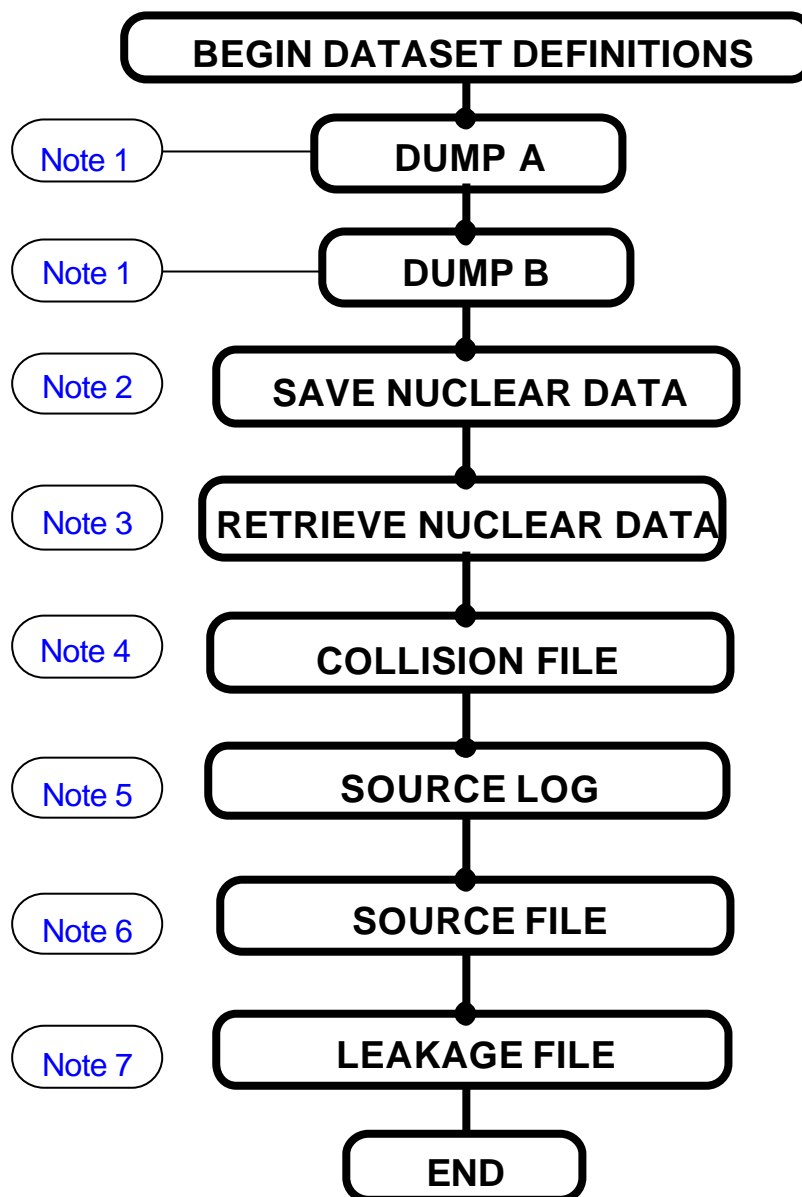
Notes

- 1 If dump(s) are required then they are requested here (alternately to files on channels DUMPA and DUMPB in the DATSETS file)
- 2 The processed nuclear data for a point-energy neutron calculation will be written to a file on channel name NCSAVE at the end of successful STAGE TWO processing for use in a subsequent calculation with identical materials.
- 3 Processed nuclear data for a point-energy neutron calculation will be retrieved from a file on channel name NCSAVE.
- 4 Details of collision events will be recorded during the calculation to a file on channel name CLOG.
- 5 Details of source particles will be recorded during the calculation to a file on channel name SLOG.
- 6 Source particles will be generated using records from a file on channel name SOURCE.
- 7 Details of particles escaping from the defined system via a free boundary will be written to a file on channel name LLOG.

Back Compatibility

Old style input that makes use of channel numbers, for example **COLLISION FILE 45**, is still accepted. The code ignores the user supplied channel number and continues as if only the keywords **COLLISION FILE** had been encountered.

Dataset Definitions



Examples

B3 Transport Flask, neutron collision case

```
BEGIN DATASET DEFINITIONS  
COLLISION FILE  
END
```

B4 Transport Flask, secondary gamma-ray case

```
BEGIN DATASET DEFINITIONS  
SOURCE FILE  
END
```

3.1.3 Output Control

Summary This unit is used to request extra output or to suppress the output of items normally printed.

Use This unit is optional.

Methods In the Scoring Data Unit a number of scoring items may be requested. Some of these produce copious quantities of output. In a series of dump/restart calculations it may be desirable to request the evaluation of certain scored items but to suppress their output until later in the dump/restart sequence. Flags may be set in this unit to perform this function.

In a calculation using splitting, the code will by default monitor the flow of particle fragments into each importance region and each energy group. This INFLOW data is printed at the end of the calculation and may be used to monitor the efficiency of the supplied importance map. If this data is not required its evaluation may be suppressed via this unit.

If the code is requested to record the details of collision events to a file defined in Dataset Definitions Unit then, by default, all events are recorded. It is possible to restrict the records to specific reactions with specific nuclides in nominated materials, e.g. record capture events in iron occurring in stainless steel.

For diagnostic purposes a printed record may be requested of all the events which take place during particle tracking. This lengthy output would normally be restricted to a few particle histories.

MCBEND is written as a series of numbered modules in the WRMS modular programming scheme and stores the bulk of its numerical data in a large database. The contents of this database may be printed at the end of the calculation. It is also possible to request a print of the data pertaining to particular modules at key points in the processing. These facilities are principally used for program development and debugging but may be of occasional use to the user familiar with the WRMS system.

Relationship with other units

Control Data The query print begins at a nominated sample and can apply to all samples taken up to the end of the calculation. The sample limit requested in Control Data Unit should not be too far beyond the initiation of a query print if massive output files are to be avoided!

Dataset Definitions If specific collision combinations are requested then a collision file should be assigned in Dataset Definitions Unit.

Scoring Data The suppression of the print of scored items should logically be consistent with the scoring requests in the Scoring Data Unit but inconsistencies will not prevent execution.

Notes on Sheet 1

- 1 Output of scored items may be deferred until later steps in a sequence of dump/restart calculations. Suppression of **INFLOWS** is a special case and refers to the monitoring of particle fragments in the importance map. If suppressed, inflows are not evaluated and cannot be 'reactivated' later in a dump/restart sequence.
- 2 If collisions are to be recorded on file during execution then the default is to record all events. This section allows the records to be restricted to specific events.
- 3 The record of collisions may be restricted to those occurring below the energy ECOLL.
- 4 The characteristics of a collision event include:

MATNO	The material number in which the collision occurs:
LDFN	The DFN (see Chapter 4, Appendix B) of the nuclide (Note that these should be the appropriate temperature dependent DFNs for a temperature dependent calculation):
LPCN	The PCN (see Chapter 4, Appendix A) of the reaction type.

Combinations of these parameters may be input to restrict the collision records. A value of 0 for any parameter signifies 'any'. Negative PCN values may be used to denote exclusion of a particular reaction type. Thus:

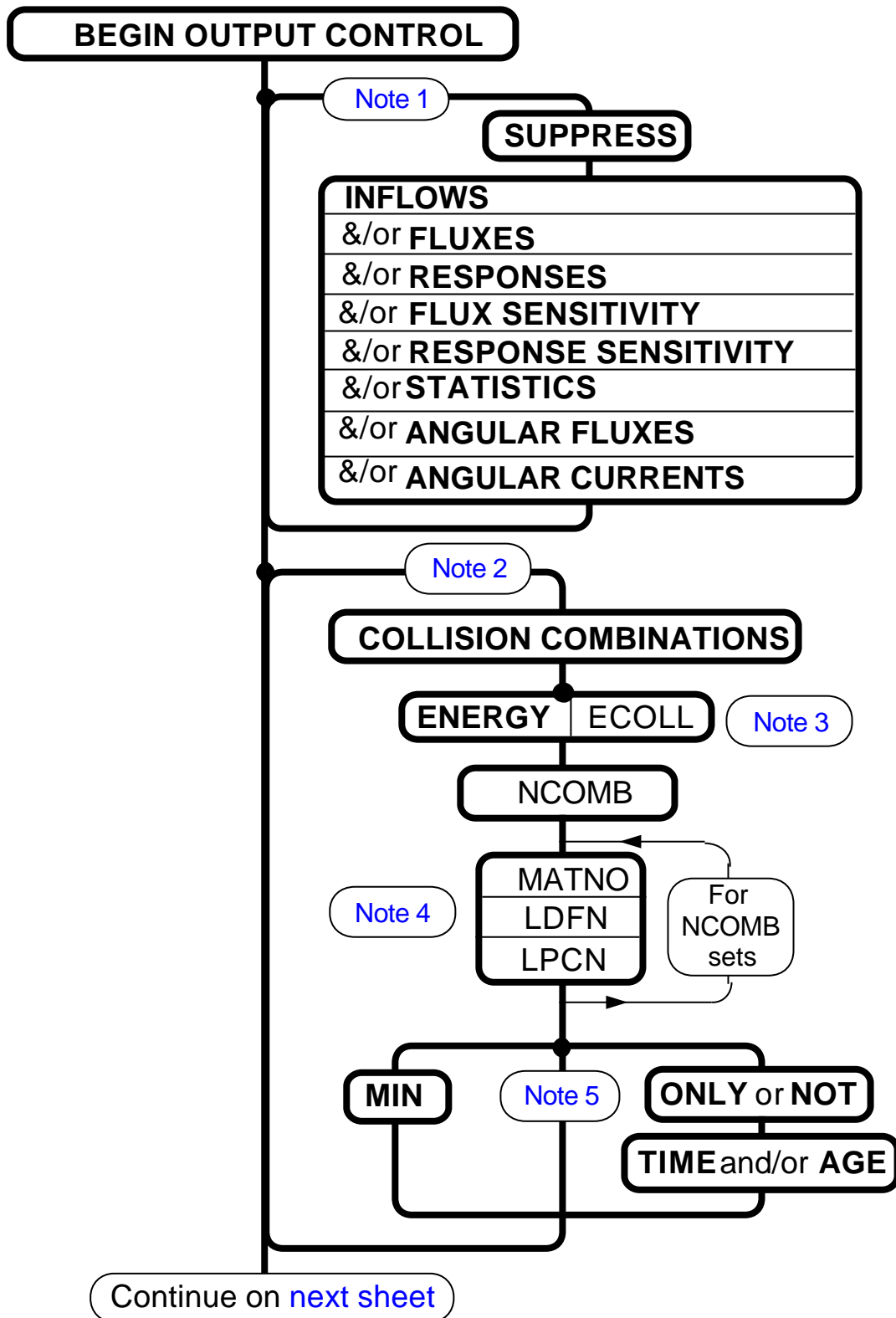
MATNO = 1 ; LDFN = 0 ; LPCN = 0 signifies ' any collision in material 1 '

MATNO = 0; LDFN = 0; LPCN = -2 signifies 'all collisions except for elastic scatter (PCN 2)'. An alphanumeric name may be used for MATNO as an alternative to a material number.

Generally the user should restrict the collision records to limit the size of the collision file. In particular, elastic collisions are rarely required for further processing and, since they are numerous, recording them will quickly produce a very large file; thus they should normally be excluded.

The number of combinations to be defined is specified by the variable NCOMB.

- 5 The **MIN** keyword requests a reduced set of collision parameters (i.e. it excludes the **TIME** and **AGE**) in order to reduce the output file size. Either **TIME** or **AGE** may be included by specifying **ONLY** followed by the required parameter - this will add the required parameter to the **MIN** set. Alternatively **NOT** may be specified to remove **TIME** or **AGE** from a full set of parameters. Inclusion of both **ONLY** and **NOT** is to allow for expansion of this option in the future.



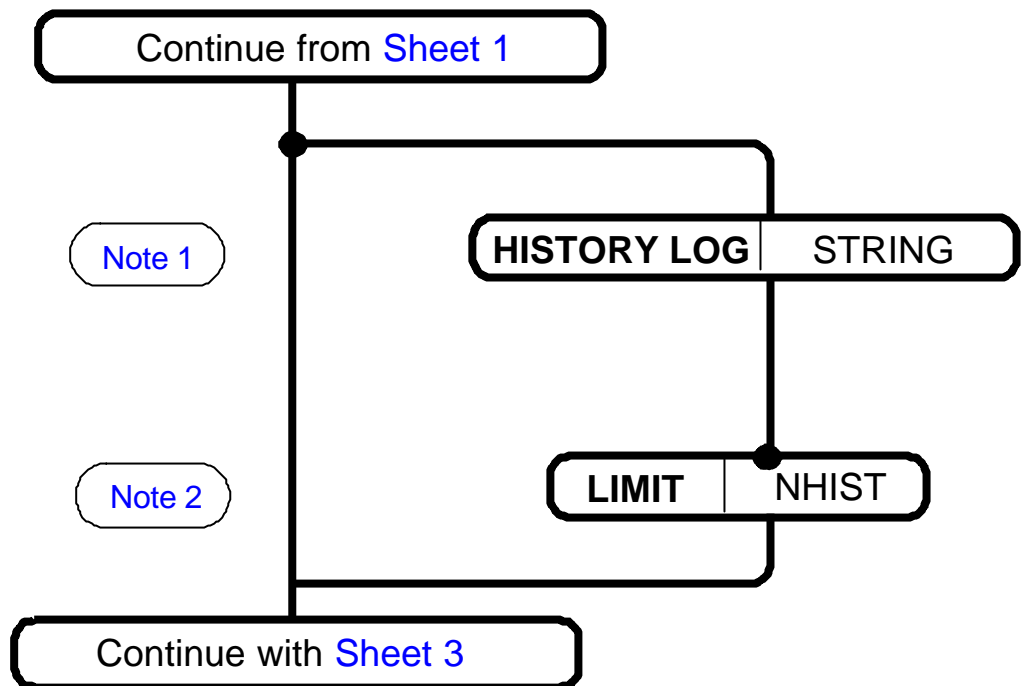
Notes on Sheet 2

- 1 The request for a log of particle histories to be made begins with the keywords **HISTORY LOG** followed by a string of letters identifying the properties that are to be recorded for every event. The options are as follows.
 - E The energy of the particle.
 - W The particle weight.
 - T The time at which the event occurs.
 - M The material in which an event occurs.
 - Z The zone in which an event occurs. The part number is also recorded.
 - R The scoring region in which an event occurs.
 - D The DFN number of a collision.
 - P The PCN number of a collision.

For example the string EWR requests the recording of particle energy, weight and the regions in which the events occur. The letters in the string may be in upper or lower case and in any order. No gaps are allowed. The example string could be extended to request the event time by adding 'T' on the end. Particle energy is always recorded, even if omitted from the string. If no other results are required then E is effectively a null string.

- 2 The number of recorded histories may optionally be limited. The number of histories (NHIST) will not, in general, correspond to the first NHIST samples since the log is restricted to those samples that include a scoring event. If collision file sources are used, the history count is increased for each point from the collision file that produces a score rather than being increased with each sample number. A value for NHIST between 50 and 100 is adequate for most purposes.

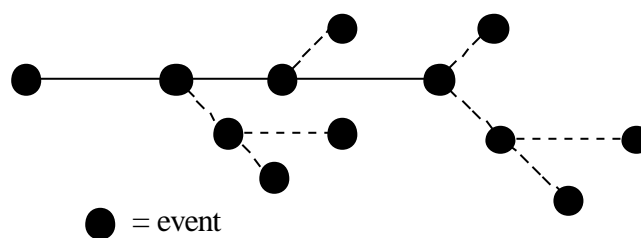
Sheet 2 : Output Control



Explanation of the History Log

A particle history is made up of straight line tracks between successive events. In the context of this history log, an event is a source point, collision site or an escape from the system. Boundary crossings are not recorded since they do not change the direction of a track or the properties of the particle travelling along it

An entry in the history log file is a set of tracks between events. The tracks usually form a branching structure caused by splitting and the production of multiple secondary particles at collisions.



The tree is pruned back to the last scoring event on each branch before being written to file. The history log file records the locations of the events, their properties and a description of how they are joined by particle tracks.

A particle history log is written to an unformatted file assigned by the user to the named channel HLOG in the DATSETS file.

The history log is for use with post processing packages for display and/or analysis of the tracks. Refer to the VISTA-TRACK user guide for more information.

Notes on Sheet 3

Note that all of the facilities on Sheet 3 are provided for programmer use. They are included here for completeness.

- 1 A request for a query print log of tracking events which happen to all samples in the range NSTART to NSTOP inclusive. If NSTOP<NSTART then query printing will continue until the end of the run.
- 2 The query print may be restricted to a maximum number of events (the first NEVENT events) for any sample. The default value for NEVENT is 100,000.
- 3 The query print may be set to include only certain events or to exclude certain events. LIST is a list of event identifiers for inclusion or exclusion. These event identifiers are numeric values and are listed below:-

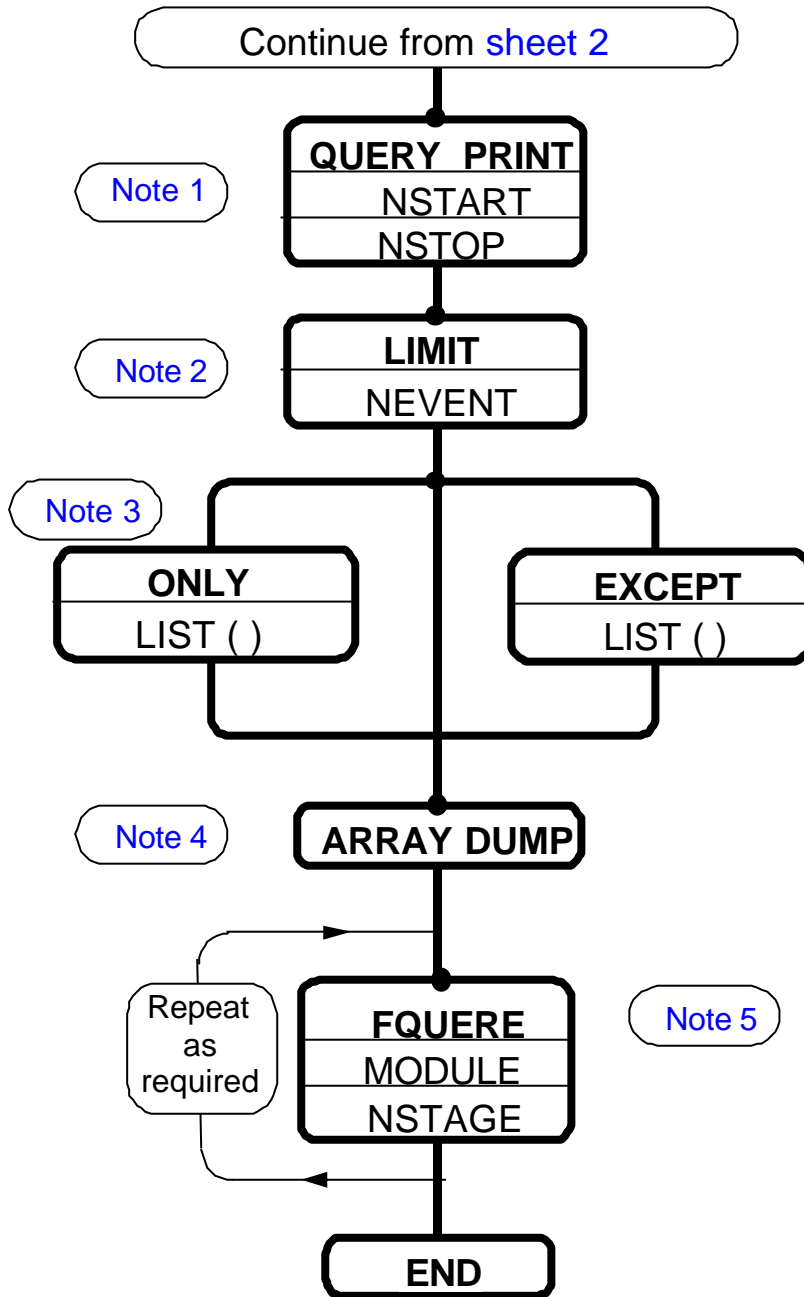
- | | |
|----|--|
| 01 | A new sample has been started |
| 02 | Distances to boundaries (zone, split, time) and collision |
| 03 | Returned from tracking after track initialisation |
| 04 | Crossed a material (=FG ZONE) boundary |
| 05 | Crossed a combined material/splitting boundary |
| 06 | Crossed a splitting (importance) boundary |
| 07 | Crossed a time zone (time dependence case) boundary |
| 08 | A collision has occurred (gamma or neutron) |
| 09 | Escape at boundary or energy<cutoff or time>TMAX |
| 10 | Absorption at collision |
| 11 | Get value of mean-free-path for current material |
| 12 | Albedo surface |
| 13 | Collision of charged particle |
| 14 | A pseudo collision has occurred in a hole material |
| 15 | Splitting/roulette (S/R) at boundary crossing |
| 16 | Charged particle boundary crossing |
| 17 | Post collision parameters of scattered particle |
| 18 | Result of S/R for scattered particle |
| 19 | Collision parameters (DFN,PCN) returned by DICE |
| 20 | Particle retrieved from the splitting bank |
| 21 | Outer boundary reflection (specular, isotropic or \cos^2) |
| 22 | Periodic boundary condition |
| 23 | Forced flight interface |
| 24 | Stack contents in detailed PHD scoring |

- 4 A dump of the entire WRMS modular system database may be requested by using these keywords. The dump is generated at the end of the calculation. This option is provided principally for programmer use.
- 5 Dumps of the WRMS data base relevant to particular modules may be requested for debugging purposes. MODULE is a module number; the module numbers and their functions are listed in the MCBEND output header. NSTAGE signifies when the dump is to be given:

- | | |
|------------|---|
| NSTAGE = 1 | : after reading the input data |
| NSTAGE = 2 | : after cross-checking the complete input data |
| NSTAGE = 4 | : after initialisation but before sampling begins |
| NSTAGE = 8 | : at the end of the calculation. |

Sums of these values are used to give multiple dumps. E.g. 9 = 1 + 8

Sheet 3 : Output Control



Examples

B3 Transport Flask, neutron collision case

```
BEGIN OUTPUT CONTROL
SUPPRESS INFLOWS
COLLISION COMBINATIONS 1
0 0 -2                ! Record all non-elastic collisions
END
```

B4 Transport Flask, secondary gamma-ray case

```
BEGIN OUTPUT CONTROL
SUPPRESS INFLOWS
END
```

Further Examples

1 BEGIN OUTPUT CONTROL
SUPPRESS INFLOWS STATISTICS
QUERY PRINT 1000 1100
END

2 BEGIN OUTPUT CONTROL
SUPPRESS FLUXES ! Do not print scored fluxes
COLLISION COMBINATIONS
ENERGY 0.01 ! Record collisions only below 0.01 MeV
3 ! 3 collision combinations will be defined
0 908 0 ! Any reaction with Fe in any material
St_steel 446 0 ! Any reaction with Cr in a material with
! alphanumeric name 'St_steel'
1 0 102 ! (n, γ) reactions with any nuclide in material 1
END

3 BEGIN OUTPUT CONTROL
ARRAY DUMP ! Print database at end of calculation
FQUERE ! Print module 0 data groups at all stages.
0 15 ! (note: 15 = 1 + 2 + 4 + 8)
FQUERE 25005 2 ! Print tracking module data groups
! after input checking
END