SPALLATION NEUTRON SOURCE PROJECT
OAK RIDGE NATIONAL LABORATORY

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Neutron Source Systems Development – WBS 1.1.4

WP No. 1.1.4 Neutron Source Systems Development

Activity: TG01040272 – Initiate development of the CALOR-DOORS interface coupling code (Phase I)

Milestone: TG01040274 – Issue report on status of CALOR-DOORS interface coupling code development (Phase I).

Monte Carlo to Discrete Ordinates Coupling Code Development

1. Introduction

Radiation transport calculations can practically be done either with Monte Carlo codes or with Discrete Ordinates codes both having strengths and weaknesses. The Monte Carlo method is perfectly suited to accurately model the physics of many interacting particle types in complicated three-dimensional problems. The limits of this method are in statistics. By extracting flux results from the tracks of a limited sample size of particles, it is often difficult to obtain a sufficient particle population far away from the source with many mean free paths of material to penetrate. Furthermore, flux results can usually be accessed only at a restricted number of locations without paying the penalty of a significant increase in computational time. The Discrete Ordinates method has its big strength in deep penetration. However, really big three-dimensional problems consisting of millions of mesh cells are still beyond the capabilities of the ordinary engineer's computer. The Discrete Ordinates method is in principle not limited to neutral particle transport but very little work has been done to extend the codes and data to charged particles. Consequently, the domain of Discrete Ordinates is neutron and photon transport. The conclusion that the Discrete Ordinates codes are powerful where the Monte Carlo codes fail and vice versa is the strongest argument to develop a coupling tool that allows the analyst to split a problem into sub-problems and to solve the sub-problems with the method of choice.

The task of coupling Monte Carlo particle transport to Discrete Ordinates transport consists of two parts, the coupling of Monte Carlo to Discrete Ordinates and the coupling of Discrete Ordinates to Monte Carlo. Applications of the first part typically arises when a shielding analysis has to be performed for an accelerator target station design. The Monte Carlo transport codes are well suited for modeling the geometrical details of the target and the physical complexity of the particle interactions and tracking. At some distance from the target the charged particles have ranged out and neutrons and photons dominate. Here an interface file of particle crossing events has to be created by the Monte Carlo code that, after having been transformed into the correct format by a coupling code, can be picked up by a discrete ordinates code to complete the radiation transport and produce reliable flux and dose level answers even in large distances of shielding material. Application of the second part of coupling comes into play when a complicated geometry like a hot cell is located behind a bulk shield and detailed flux and dose levels are required in this cell. In this case a flux file originating in a two or three-dimensional discrete ordinates calculation is very likely available. The analyst can extract a boundary flux distribution from the flux file and provide it to a Monte Carlo calculation in order to solve for dose levels utilizing the geometrical details in the hot cell.

The first type of coupling is addressed with priority, because urgent SNS shielding problems are already waiting to be solved. The second part of coupling will be addressed later. A detailed investigation has been performed to identify the interfaces for coupling Monte Carlo calculations to Discrete Ordinates calculations. These interfaces are more fully described in the next section. The DOORS package comprises Discrete Ordinates transport codes for one-, two and three-dimensional problems. Because it is beyond the project to provide a coupling tool for all possible modes of operation of these codes, a reasonable subset of modes has been defined that will be covered by the coupling tool. This subset is described in Section 3. The first pieces of coupling code are being written to transform the MCNP type surface source file into a two-dimensional R-Z DORT boundary source file. Details are presented in Section 4.

2. The Interfaces of Coupling Monte Carlo to Discrete Ordinates

The work package asks for a tool to couple the CALOR and DOORS code systems. The CALOR code system basically employs the HETC code for charged particles and high energy neutron transport, the MORSE code for the low energy (below 20 MeV) neutron and gamma transport and the EGS4 code for electron and gamma transport. To avoid elaborate multi-group cross section generation, the MORSE code has been replaced by the MCNP4B code that uses a different geometry package. The upgrade of the HETC and EGS4 codes with the MCNP geometry package has been completed recently and enables the analyst to use the same geometry description for all Monte Carlo codes.

Many of the nuclear designers, however, use the LCS code system or the MCNPX code to perform the high energy transport part of the calculations. The LCS code system uses the LANL derivative of HETC, LAHET, for the high energy transport, the post processing code PHT for generating the gamma sources from the residual nuclei, and the MCNP4B code for the low energy neutron and gamma transport. The MCNPX code combines the LCS codes used for the high energy transport with the MCNP4B code for the low energy neutron and gamma transport.

To provide a tool for all nuclear designers the objective of the task has been extended to provide a tool for coupling the CALOR, LCS and MCNPX codes with the DOORS code system. The additional effort is minor as will be seen later. Hence, the tool to be generated has to prepare interfaces from the high energy Monte Carlo codes HETC, LAHET and MCNPX and the low energy (below 20 MeV) code MCNP4B to the discrete ordinates codes TORT, DORT and ANISN of the DOORS package working in three, two and one dimensions, respectively.

2.1 The Monte Carlo Boundary Crossing Interfaces

Except for the HETC code, all transport codes involved are released in frozen versions. All the frozen codes, LAHET and the MCNP variants, provide an interface that can be accessed for coupling the Monte Carlo codes to the codes of the DOORS system. This allows the analyst to use the codes in their standard versions and eases quality assurance. The HETC code has been updated to be able to provide an interface.

From the Monte Carlo side the interface is the information of particle boundary crossings that are reported to a history file. This history file will later be analyzed to give boundary flux information for the discrete ordinates codes binned by space, angle and energy. To limit the storage space, only boundary crossings at defined surfaces, e.g. the Monte Carlo - Discrete Ordinates (MC-DO) interface, need to be saved on a history file. The history file formats for the different codes and the information stored on the files is summarized in Table 1 and explained in the following paragraphs.

Table 1: Types of boundary interface files of the Monte-Carlo codes.

Monte Carlo Code	Interface File Format	Boundary Crossing Information
HETC	LAHET type HISTP	internal boundary crossings particle escape
LAHET	LAHET type HISTP	particle escape
MCNPX	MCNP type SSW	internal boundary crossings particle escape
MCNP4B	MCNP type SSW	internal boundary crossings particle escape

Principally two physical events are of use as interface information, internal boundary crossings and particle escape events. The MCNP type codes have a surface source writing and reading capability implemented that enables a very flexible specification of surfaces and the particle types for which information is to be saved. The LAHET code allows the analyst to specify the particle type, and the event type including internal boundary crossing and particle escape. However, because LAHET lacks the ability to define specific boundary surfaces and therefore writes boundary crossing events for all boundary crossings, the event specification ``internal boundary crossing'' is of limited use. The event specification ``particle escape'', however, is very well suited for defining boundary crossing information.

As mentioned before, HETC was extended for this task to include the LAHET type specification scheme. In addition, an option was implemented to define interface surfaces for boundary crossings, so that ``internal boundary crossing'' and "particle escape" events can utilized as boundary interface information. In the same effort an option was implemented into HETC to switch from the HETC type format of the history file to the very similar LAHET type of the history file, cutting down the number of different interface file formats from the Monte Carlo side to two.

2.2 The DOORS Boundary Source Interfaces

The DOORS code system provides ANISN, DORT and TORT transport codes for one- two- and three-dimensional problems. Although the codes are distributed in one package, each code has its own conventions and file formats to treat boundary sources.

The ANISN code:

The ANISN code can operate in three modes: the spherical, the infinite cylindrical and the infinite planar mode, all of which have their importance in for specific shielding cases. It offers two types of source specifications, the volume distributed source and the shell source. Both source types can be read only in input card form. The volume distributed source allows for energy and space dependence and assumes isotropic angular dependence. The shell source allows surface sources by energy group and angular direction for any number of shells.

The DORT code:

Typical two-dimensional problems are of R-Z cylindrical symmetry. R-Theta and X-Y shielding problems are very infrequent and are excluded as coupling options unless a real need arises. DORT offers external and internal boundary sources as source options. The external boundary source conditions for each geometry boundary is chosen by the boundary condition flags IBL(left), IBR(right), IBT(top) and IBB(bottom). The boundary source information is passed to the code through a file in the BNDRYS format linked to the FORTRAN unit NTBSI. This option is to be used when a boundary flux is provided at the outer surfaces of a cylinder. The internal boundary fluxes are applied by setting the input parameters NJNTSR and NINTSR to the number of internal boundary sources required in the dimensions J(radial) and I(axial), respectively. The information is passed to the code at the unit number NTIBI by a file again in the BNDRYS format. The boundary source file contains boundary flux data sets bined in energy groups, spatial mesh and direction bin for each required internal or external boundary surface. External and internal boundary sources can be provided simultaneously through different files.

The TORT code:

The typical TORT geometries are of X-Y-Z box shape although R-Theta-Phi cylindrical problems can principally be solved. The latter has rarely been used and is not considered in this project. TORT offers, similar to the DORT code, the options of internal and external boundary sources. The external boundary sources are chosen by the value 4 of the flags IBL(left), IBR(right), IBI(inside), IBO(outside), IBB(bottom) and IBT(top). The information is passed to the code by a file in the VARBND format linked to the FORTRAN unit number NTBSI. Internal boundary sources are supplied by setting the parameters NINTSR, NJNTSR, and NKNTSR to the number of desired internal boundary sources. So far only the option NKNTSR (boundary at the k-planes) is supported by the code. A further crucial restriction is that the source information is provided by input cards rather than by a boundary source file. These input arrays allow the analyst to provide a shape function by direction and by the two spatial coordinates. The magnitude is given by the fission spectrum. Dave Simpson, author of the DOORS system, will address the TORT deficiencies and extend the code with the necessary capabilities.

2.3 Performing Discrete Ordinates Calculations with Monte Carlo Boundary Sources

The interface boundary condition in the Discrete Ordinates calculations has to be input differently in the cases when the code uses Monte Carlo internal boundary crossing events or particle escaping events as boundary information. Using a boundary source created from Monte Carlo internal boundary crossing events the analyst has to make sure that the angular flux contribution from the MC side of the geometry is zero. This can be realized by supplying a black absorber in the MC region in the discrete ordinates calculation. When applicable (presently only available in ANISN), an explicit void boundary condition would do the same. For boundary fluxes created from Monte Carlo particle escape events, the angular flux contribution from scattering in the inner Monte Carlo region has to been accounted for . To correct for this the Monte Carlo-region has to be modeled in the Discrete Ordinates calculation probably as a mixture of material representing the detailed Monte Carlo geometry.

3. Coupling Configurations

As already mentioned above, the coupling tool will provide boundary sources only for a subset of reasonable operational modes of the Discrete Ordinates codes needing Monte Carlo information from specifically shaped interface boundaries in some cases.

ANISN configurations

ANISN operates in the one-dimensional spherical, cylindrical and planar modes, each of which is applicable to a specific shielding application.

The typical spherical problem consists of a localized source region that is completely embedded in bulk shielding material. The radiation transport into a certain direction through the shield is considered using angular directed leakage information from the Monte Carlo calculation and provided to ANISN as a distributed volume source concentrated in a small volume (quasi point source) using the preset isotropic angular distribution. The source information can also be provided to ANISN as a surface shell source that allows the analyst to model a more realistic angular source distribution. In this case, the Monte Carlo interface would preferably be of spherical shape. Sampling for the ANISN shell source could be reduced to any section of the Monte Carlo sphere to model peak leakage into the shield.

A typical application of the ANISN cylindrical mode is the shielding of a particle beam line loss, which is a very small fraction of the beam current. The line loss is usually measured per line length. The lost beam interacts with the structural material of the accelerator. This line loss can be modeled by the beam loss hitting a target producing secondary particles through a Monte Carlo calculation. Shielding calculations for an accelerator line is easiest done in the Monte Carlo calculation by scoring the integral leakage of the interacting beam at the surfaces of a cylinder and continue with a ANISN calculation in the cylindrical mode with the leakage information used as quasi line source with isotropic angular distribution. More detailed angular information can again be provided to ANISN using a shell source.

A spatially extended beam may produce a radiation field that impinges on a large area of a shielding wall. Such a case is dedicated to ANISN in the planar mode. A Monte Carlo calculation would model the fraction of the beam impinging on a unit area, and score the boundary crossings at a plane perpendicular to the beam in angle. This information is fed into ANISN as a thin layer distributed source in isotropic angular distribution or as a shell source in a detailed angular distribution.

DORT and TORT configurations

DORT coupled calculations are only considered to be of cylindrical R-Z geometry, TORT problems are considered to be only of box shaped X-Y-Z geometry. The Monte Carlo boundary interface is expected to be of the same shape as the shape of the coupled geometry. External and internal boundary sources are provided to DORT/TORT by different file formats and need therefore to be treated as different cases. Also, degenerate boundary interfaces might appear when the DORT/TORT model only partially overlaps with the Monte Carlo model. In the extreme case, when the Monte Carlo and the Discrete Ordinates models are attached to each other but do not overlap, the Monte Carlo interface is a plane rather than a cylinder or box.

4. The Realization of the MCNP(X) to DORT coupling code

Driven by the need to start energy deposition calculations for the bulk shielding surrounding the mercury target, a conversion tool is in development that will allow the analyst to use surface crossing files in the MCNP SSW format to initialize DORT R-Z boundary source terms. This tool will enable the analyst to use the results of MCNP calculations (or of any other code that compiles the same type of surface crossing information in SSW-like files) to couple to DORT calculations of adjacent or overlapping problem regions as sketched in the previous section.

At the current time, the coding has been completed for reading the MCNP SSW type of surface crossing file, binning the particle information into the discrete spatial mesh, energy groups and angular quadrature, and create a DORT boundary flux file of BNDRYS format. This boundary flux file couples standard MCNP neutron/photon problems with DORT for both adjacent and embedded MCNP calculations. Two simple sample problems have been run to verify the methodology; both of them involve very thin shields (about one mean free path) so that a full solution can be generated with MCNP for comparison in a reasonable time. The results agree within 10%. In reality, of course, the method will be primarily useful for thick shielding situations.

The next programming steps will be to extend the code first for the MCNPX SSW type (differs slightly from the MCNP SSW format) and then for the LAHET HISTP type of boundary source files.