# NRC User Codes for EGSnrc

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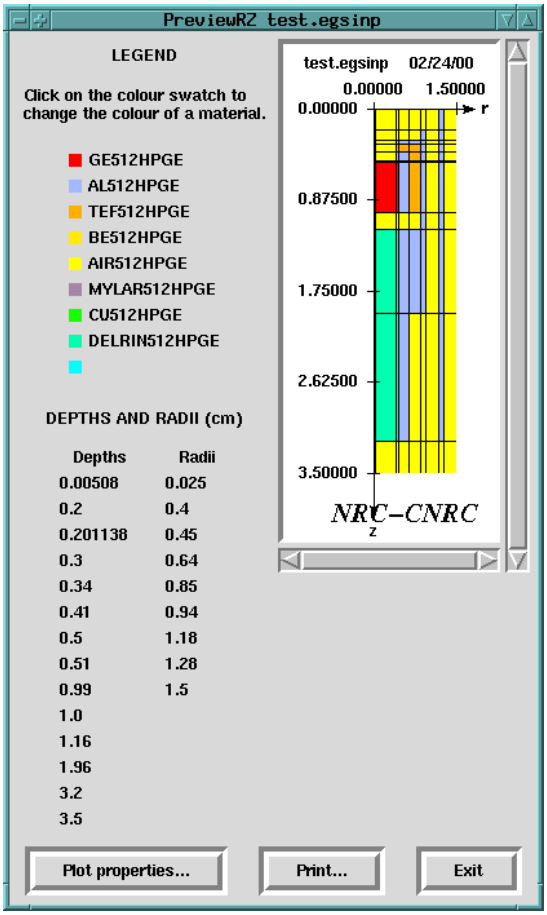
**April 3, 2019**

NRCC Report PIRS-702(revC)




Preview of an RZ geometry in DOSRZnrc.

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**Abstract**

This manual describes the NRC User codes DOSRZnrc, CAVRZnrc, FLURZnrc and SPRRZnrc which all work with the EGSnrc Code system for Monte Carlo transport of electrons and photons (see NRC REPORT PIRS–701, "The EGSnrc Code System"). There is a graphical user interface available for creating the inputs to these codes (described separately).

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# 1 Introduction

## 1.1 Intent of this report

Over the years, NRC has developed and distributed a series of user codes for use with the EGS4 code system for the Monte Carlo simulation of photon and electron transport. These have been widely used and their results compared to experiment in many cases. However, the codes themselves have never been properly documented and described. It is the purpose of this manual to provide a document which describes both how these codes work and also how a user uses them. It is not the purpose of this manual to discuss selection of parameters when using these codes for a particular application since this is a huge undertaking and is covered in the already extensive literature on EGS.

Recently, the codes have been reworked to use the new EGSnrcMP system[1]. This has increased the flexibility of these codes, including the ability to run them on both Unix/Linux and Windows systems.

The codes involved in this report are all for cylindrical RZ and spherical geometries. These are:

**DOSRZnrc** which scores dose in a generalised cylindrical geometry.

**FLURZnrc** which scores particle fluence in the same geometry.

**CAVRZnrc** which is similar to DOSRZnrc but also scores a variety of quantities which are of specific interest to dosimetry calculations for an ion chamber.

**SPRRZnrc** which calculates Spencer-Attix spectrum averaged stopping-power ratios for arbitrary media.

**CAVSPHnrc** which is identical to CAVRZnrc but for spherical geometries.

**EDKnrc** which calculates energy deposition kernels for photons or electrons forced to interact at the centre of a spherical phantom. It can also calculate dose distributions in the entire phantom or the dose to specific regions defined as the cavity of a spherical ion chamber.

This manual does not describe the BEAM code for modelling radiotherapy accelerators, $^{60}$Co units and x-ray systems. BEAM is described elsewhere[2, 3]. The user codes described here all have the capability of using either a BEAM generated phase space file or a full BEAM simulation (compiled as a shared library) as the source of incident particles.

Also, this manual does not describe the EGS_Windows system for doing 3D displays of EGS simulations. EGS_Windows is described in detail in its own manual[4].

## 1.2 History

These codes have a long history at NRC and were first written to work with EGS3 which was written in Mortran2. The first germs of these codes were written by Alex Bielajew who was

responsible for coding CAVRZ as a research tool for work related to ion chamber dosimetry. This then grew into DOSRZ which strips out some of the special purpose parts of CAVRZ but adds various more general purpose facilities such as calculating response functions for detectors. Dave Rogers took these codes and developed a general purpose fluence scoring code FLURZ and finally SPRRZ was developed. Along the way various summer students worked under Dave Rogers and Alex Bielajew to add features.

One problem was that all the codes had grown on their own with various bits and pieces being patched in whenever they were needed for a particular research project. The system of codes was getting more and more difficult to maintain and various options failed to work on new systems as they came along (eg the output listing from FLURZ didn't work on Unix systems because it was based on a Digital Vax Fortran extension which was not commonly available on unix Fortran compilers). This was overcome in the DOSRZ code by some horrific coding tricks which made it impossible to change the outputs. Furthermore the input files became almost impossible to create since they were just a large file of numbers where the meaning of each number was dependent on its position, and often meant different things for the different codes.

To overcome these shortcomings, a major revamping was undertaken in 1998 by Aaron Merovitz, a summer student working for Dave Rogers. Firstly he created some general purpose output routines which worked for standard compilers. Also, as much as possible all graphical output was done through a single subroutine called `xvgrplot` so that if changes in plotting output are required. it needs to be changed in only the subroutine. Next a text based system for input files was written which is much easier to use than the previously used long string of numbers. This tool was then used to create a single routine to read geometry inputs for all the user codes so that now one can cut and paste the geometry description from one user code to another. This was extended for source routines and transport routines so that the input files start to look similar for all the user codes. More importantly they are much easier to read and know exactly what the simulation is about without having the description of the inputs open on your desk.

In 1999, the codes were upgraded to use the then-new EGSnrc code system. This was done by Iwan Kawrakow with Jan Seuntjens and Dave Rogers. In the process many small bugs have been found and fixed.

In 2002, Ernesto Mainegra-Hing developed a very powerful C++ graphical user interface which is based on the Qt(version 3) system[5].

The final major upgrade has been to make the codes work with the new EGSnrcMP code system. This has been undertaken by Iwan Kawrakow with support from Ernesto Mainegra-Hing and Blake Walters.

In the individual descriptions below of the codes we cite various specific references to papers in which the various aspects of the code have been described.

As the above history makes clear, these user codes have been developed by many different people over a long period of time, and the codes have all benefited by extensive feedback and bug patches from the user community. In particular, we wish to recognise the contribution of Alex Bielajew to the development of these codes over a long period of time while he was at NRC.

# 2 Common Features of All Codes and Associated Inputs

## 2.1 Subroutines in the RZ codes

As pointed out before, all NRC RZ-codes work within the same RZ geometry, and their `HOWFAR` and `HOWNEAR` routines are exactly the same. Most of the other common subroutines and macros have been split off as much as possible (but not completely) from the user code file. They include:

- random number generators (`ranmar.macros`, `ranmar.mortran`, `ranlux.macros`, `ranlux.mortran`)
- machine specific macros / routines (`machine.mortran`)
- EGSnrc specific macros and routines (`egsnrc.mortran`, `egsnrc.macros`)
- RZ geometrical subroutines (`geomrz.mortran`)
- input parser routines (`get_inputs.mortran`, `transportp.macros`)
- Sources and energy sampling routines available for the RZ codes (`srcrz.mortran`, `ensrc.mortran`, `srcrz.macros`, `phsp_macros.mortran`)
- `IWATCH` output routine (`nrcaux.mortran`)
- Routine to output RZ grid to `.egslst` file (`grids.mortran`)
- Routines for initializing data I/O, opening output files, etc (`egs_utilities.mortran`)
- Routines for built-in parallel processing functionality (`egs_parallel.mortran`)

The scoring routine `AUSGAB` is fundamentally different for each of the user codes, and will be discussed later in this document.

## 2.2 Region and plane numbering convention

The numbering of the regions, planar zones and cylindrical ring zones in the RZ codes is shown in figure 1 in which the Z-axis is the axis of rotation shown by the dotted line running across the page. `NR` represents the number of cylinders or rings, and `NZ` the number of planar regions or slabs, which are defined by `NZ + 1` planes. (`IX`,`IZ`) denote the (r,z) indices of a subregion in the RZ space. The input specification of the geometry and materials is summarised in the next section.

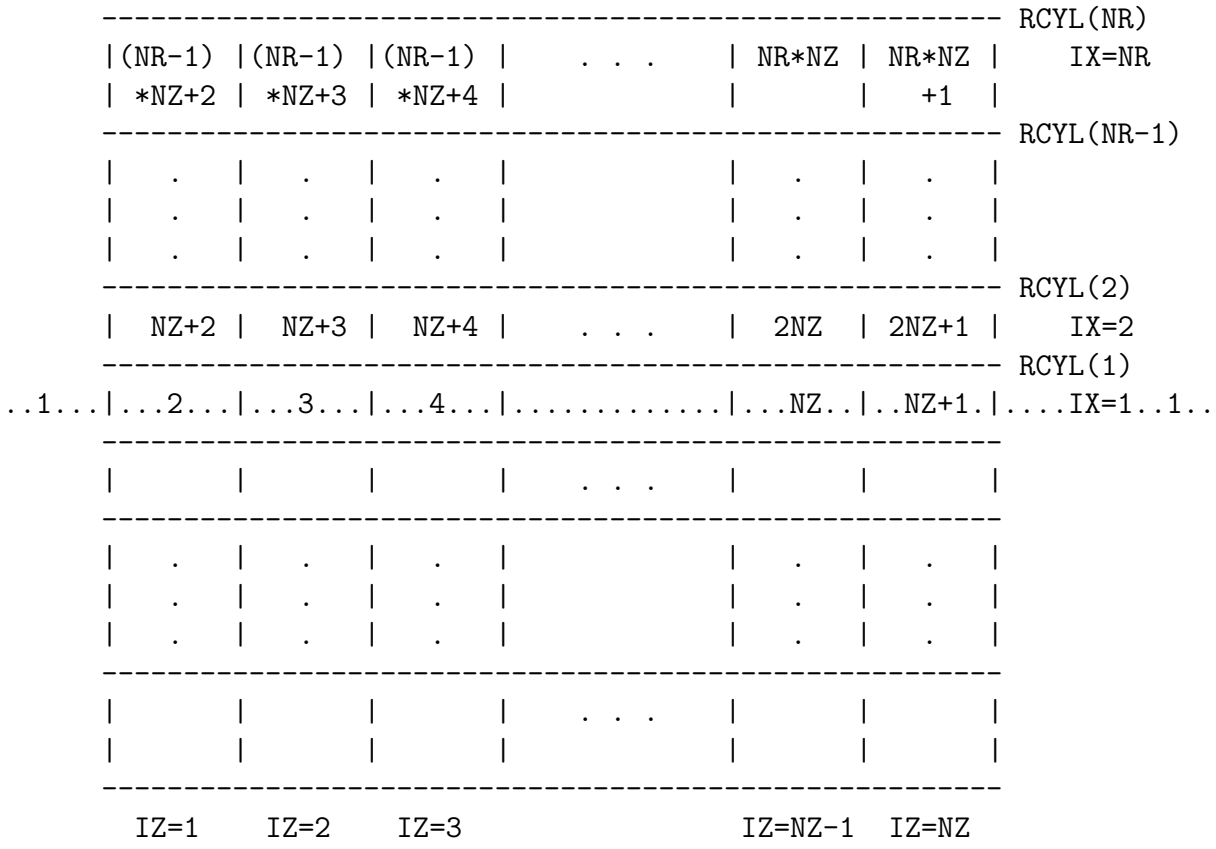


Figure 1: Geometry of the RZ NRC user codes. The dotted line is the z-axis which is the axis of rotation. The exterior of the geometry is zone 1. There are `NZ` depth slabs or regions which are defined by `NZ + 1` planar boundaries specified by `ZBOUND(1:NZ+1)`. There are `NR` radial regions or rings defined by their `NR` outer radii contained in `RCYL(1:NR)`. The region numbers are reflected in the axis of rotation.

## 2.3 Using the text based input format

The input for the RZ codes is handled by each code's INPUTS subroutine. It in turn makes multiple use of a common routine called `GET_INPUT`. The function is located in the file `get_inputs.mortran` and for the RZ codes it is, along with other files, concatenated before being compiled. We briefly describe the use of the function `GET_INPUT` for implementation in user codes.

`GET_INPUT` will extract the requested `values_sought` from the input file and return it to the caller. Inputs are all in the format:
`name of value_sought= value`
where `name of value_sought` must match that expected by the program. Example of typical inputs handled by `GET_INPUT` are:

```
MEDNUM= 0, 1, 2
MEDIA= AIR700ICRU
RAYLEIGH SCATTERING= on
```

The rules governing the use of the `GET_INPUT` routine are:

- The `value_sought` must be the first thing on a line but blanks are allowed before it.
- The `=` sign must have no blanks between it and the text for the `value_sought` and at least one blank before the value input.
- Various inputs are only sought between certain delimiter strings which are defined below (*e.g.*, `:start I/O control: :stop I/O control:`) If the delimiter string is not specified, the whole file is searched for a requested `value_sought`.
- Delimiter strings are enclosed by colons.
- Within delimiter strings, order of inputs does not matter.
- If a requested quantity is not found, this is noted in the file `$input.errors` and this file is printed at the end of the log file.
- A semi-colon implies the end of input for this quantity but is not mandatory. This means that semi-colons cannot be used in titles.
- A `#` sign indicates that everything else on the line is a comment (do not use in titles).
- Commas separate multiple values for a given quantity and a comma at the end of a line implies there is more input on the next line.
- There can be coupled multiple inputs whereby the first value of some `value_sought` is associated with the first value of some other `value_sought` and possibly with the first value of a third `value_sought`, etc.
- Values can extend over as many lines as needed. Use commas to imply there are more values on the next line.
- Blank lines and blanks in general are ignored.

- The maximum record length is 256 characters.
- Inputs are not case sensitive.

### 2.3.1 Using GET_INPUT

This section is only of interest to those wanting to modify the user codes or add a new input.

There are 4 types of inputs defined: type 0, REAL numbers; type 1, INTEGERs; type 2, arbitrary character strings (eg titles); type3, predefined character strings, or "allowed inputs".

To implement GET_INPUT one must first establish a set of requested inputs and then make a call to get_input for one or more inputs (which are specified by a counter).

The following summaries the implementation of GET_INPUT for different types of input.

```
            REALS AND INTEGERS (TYPE 0 AND 1)
I=I+1;                                <--index counter
NUM_DRMIN=I;                          <--named pointer to the index num.
VALUES_SOUGHT(I)='DOSE RBOUND MIN'; <--name of variable
NVALUE(I)=1;                          <--# of inputs(left out if not known)
TYPE(I)=0;                            <--Type (0-3)
VALUE_MIN(I)=0;                       <--Minimum value
VALUE_MAX(I)=$MAXRADII-1;             <--Maximum value
DEFAULT(I)=0;                         <--Default value

            CHARACTER INPUTS (TYPE 2)
I=I+1;
NUM_TITLE=I;
VALUES_SOUGHT(I)='TITLE';
TYPE(I)=2;
NVALUE(I)=1;                          <--left out if not known

            ALLOWED INPUTS (TYPE 3)
I=I+1;
NUM_IWATCH=I;
VALUES_SOUGHT(I)='IWATCH';
NVALUE(I)=1;                          <--left out if not known
TYPE(I)=3;
ALLOWED_INPUTS(I,0)='OFF';
ALLOWED_INPUTS(I,1)='INTERACTIONS';
ALLOWED_INPUTS(I,2)='STEPS';
ALLOWED_INPUTS(I,3)='DEPOSITED';
ALLOWED_INPUTS(I,4)='GRAPH';
                     **** STATE THE DELIMITER ****
          DELIMITER='TRANSPORT CONTROL'
   OR     DELIMITER='NONE';
```

For REAL and INTEGER input types, the user may specify minimum and maximum acceptable values, and if the iput is outside this range, the code uses the specified DEFAULT value. Note however that if the particular VALUES_SOUGHT is not input, then an error flag is set, an error message produced and eventually the program in terminated, i.e. the default value is not a true default.

After these parameters have been specified, call the subroutine GET_INPUT with the appropriate index number of the values_sought (use NMIN and NMAX). An example is shown below.

```
ival=1;
NUM_ESTEPE=ival;                    --> store index for ESTEPE variable
VALUES_SOUGHT(IVAL)='ESTEPE';
NVALUE(IVAL)=1;
TYPE(IVAL)=1;
VALUE_MIN(IVAL)=0.0;
VALUE_MAX(IVAL)=1.0;
DEFAULT(IVAL)=$MAX-ELOSS;

IVAL=IVAL+1;
NUM_XIMAX=IVAL;
VALUES_SOUGHT(IVAL)='XIMAX';
NVALUE(IVAL)=1;
TYPE(IVAL)=1;
VALUE_MIN(IVAL)=0.0;
VALUE_MAX(IVAL)=1.0;
DEFAULT(IVAL)=$EXACT-BCA-XIMAX;

...
NMIN = 1; NMAX = IVAL;              --> specify the range of inputs
CALL GET_INPUT;                     --> call GET_INPUT

estepe=VALUE(NUM_ESTEPE,1);         --> assign the variable using
                                        the previously stored index
ximax=VALUE(NUM_XIMAX,1);
```

### 2.3.2 Note on notation

The text based input is much clearer than the previous input based on assigned values to individual variables. The one advantage of the former system is that the name of the varable used in the source code was made explicit. To allow the user to know what the internal variable is called which is specified by a particular text input, we frequently specify the name of the associated variable in square brackets after the description of the text based inputs (eg [ ECUT ] and when appropriate, the internal values corresponding to the different options are shown.

## 2.4 The xmgr/grace plotting codes

At NRC we make extensive use of the freeware, called `xmgr` or more recently `grace` for making 2-D plots of data. Most of these user codes now create files which can be immediately plotted by this software. Since we find this software so user friendly and flexible, we encourage others to download the package and install it.

The `xmgr` code is frozen and no longer being developed. It is available at http://plasma-gate.weizmann.ac.il/Xmgr and works very well for our purposes.

There is an active group developing the off-spring of `xmgr` which is called `Grace`. It has some new features which are helpful but not essential. It is available at http://plasma-gate.weizmann.ac.il/Grace.

The NRC user codes all interface to the plotting package via a single subroutine called `xvgrplot`. The output of this routine works with either package and allows histogram or point plots, log or linear plots, error bars, labels etc, etc.

However, if you have your own plotting package which you want to use, then just write a new version of `subroutine xvgrplot` which creates an output file for your plotting software.

## 2.5 Geometry and Material Inputs

### 2.5.1 The geometry inputs

The geometry inputs are delimited by the strings: `:start geometrical inputs:` and `:stop geometrical inputs:`. There are in two distinct ways to input geometry information into the RZ user codes. The choice is specified by the assigning to `METHOD OF INPUT` either `Groups` or `Individual`. If `Groups` is selected, sets of slabs of equal thickness can be input. Based on the choice made, the code expects following additional input with all dimensions entered in cm:

```
 Only if  METHOD OF INPUT=  Groups

  Z OF FRONT FACE        (R)   start of first slab (real)
  NSLAB                  (M)   # planar slabs in a group (integers)
  SLAB THICKNESS         (M)   thickness of each slab in the group (reals)


 Only if  METHOD OF INPUT=  Individual

  Z OF FRONT FACE        (R)   start of first slab (real)
  DEPTH BOUNDARIES       (M)   geometrical z-plane coordinates (reals)

-------------------------------------------------------------------------

  Information defining radial boundaries
```

```
RADII                    (M)   radii of cylinders defining geometry (reals)
```

The NSLAB and SLAB THICKNESS multiple inputs are an example of the coupled inputs mentioned in section 2.3. So, for example, the following inputs:

```
NSLAB=           2,  5,  3
SLAB THICKNESS= 1.0, 2., 1
```

mean that there are 2 slabs of 1 cm thickness, 5 of 2 cm and then 3 of 1 cm.

Radial boundaries (the radii of the cylinders defining the geometry) are entered as reals separated by commas for a value_sought called RADII..

### 2.5.2 The Material Inputs

Each geometrical region needs a material to be associated with it. The names of the materials must be entered through the "MEDIA" input. The material name must match that in the PEGS4 dataset EXACTLY, including case. 24 characters are maximum allowed per medium and are ended by , or ;

The assignment of the media to the geometrical regions can be carried out in two ways, based on the setting of the input DESCRIPTION BY= to Regions or to Planes. If DESCRIPTION BY= Regions then the user specifies the region numbers that are to be filled with the corresponding medium. If DESCRIPTION BY= Planes then the user specifies the plane (IZ) and cylinder (IX) numbers that are to be filled with the corresponding medium.

There are two additional input options, DESCRIPTION BY= Regions + Density and DESCRIPTION BY= Planes + Density. These are similar to DESCRIPTION BY= Regions and DESCRIPTION BY= Planes respectively only now, in addition to the medium to be used in a range of region numbers or plane/cylinder numbers, the user also specifies the density of the material in that region (RHOR). These latter two options are only useful if you want the medium in some geometrical regions to have a density different than its default density. Note that when using this option, the cross-sections are properly scaled to account for the variation in density (using the RHOR feature in EGSnrc), but the density effect in the electron stopping powers stays fixed at the values appropriate to the default density (this is a minor approximation in most cases).

In all cases the entire geometry is filled with medium 1 (with default density) by default. Careful selection of what is medium 1 can significantly reduce the rest of the required input. A detailed description of the material input is shown below. The corresponding internal varible names are shown in brackets [ ].

```
MATERIAL INPUT
**************

MEDIA                (M)   material name which must match that in the
                           pegs4 data set EXACTLY, including case.
                           24 characters max per medium, ended by , or ;
```

```
 Define which media in which regions, numbering in order given above.

 DESCRIPTION BY= Regions            use the individual geometric region
                                    numbers
               = Planes             use the IX, IZ values
               = Regions + Density  same as Regions but specify medium
                                    density as well
               = Planes + Density   same as Planes but specify medium
                                    density as well
                           [DESCRIBE]

If DESCRIPTION BY= Regions

 MEDNUM              (M)   the material number (integers)
                           (MEDNUM=0 => vacuum)
 RHOR (only if DESCRIPTION= Regions + Density)
                     (M)   material density if different from default
                           (real) (if 0 then assumed to be default)
 START REGION        (M)   initial geometrical zone(irl) (integers) for
                           this medium [NREGLO]
 STOP REGION         (M)   final geometrical zone(irl) (integers) for
                           this medium.[NREGHI]
                           ( >NREGLO to input more than one zone)
                           DEFAULTS:   MEDNUM=0 FOR REGION=1 (i.e. VACUUM)
                                       MEDNUM=1 FOR REGION=2,NREG

                     These inputs should be thought of as triplets
                     (quadruplets if RHOR is also specified) of
                     MEDNUM, (RHOR,) START and STOP REGIONs which are used
                     to specify the medium numbers for all regions where
                     the medium is not the default (medium 1).

If DESCRIPTION BY=  Planes

 MEDNUM              (M)   the material number (integers)
                           (MEDNUM=0 => vacuum)
 RHOR (only if DESCRIPTION= Planes + Density)
                     (M)   material density if different from the default
                           (real) (if 0 then assumed to be default)
 START ZSLAB         (M)   initial zslab(iz) (integers)
 STOP ZSLAB          (M)   final zslab(iz) (integers)
 START RING          (M)   initial radial ring (ix) (integers)
 STOP RING           (M)   final radial ring (ix) (integers)
                           DEFAULTS:   MEDNUM=0 FOR REGION=1 (i.e. VACUUM)
                                       MEDNUM=1 FOR REGION=2,NREG
                     These inputs shpuld be thought of as quintuples
```

```
                    (sextuples if RHOR is specified) of numbers
                    which specify the medium numbers and density by
                    planar - radial regions
```

A choice between `DESCRIPTION BY= Planes` (or `DESCRIPTION BY= Planes + Density`) or `DESCRIPTION BY= Regions` (or `DESCRIPTION BY= Regions + Density`) should be made based on which is the more convenient way.

An example of the geometry input for a Germanium detector is given below. In this example the advantage of having the `DESCRIPTION BY= Planes` becomes obvious, since the region numbering in the RZ codes is such that neighbouring radial regions have quite different region numbers, and entering the materials using `DESCRIPTION BY= Regions` becomes very lengthy. Note also that between minimum and maximum plane and between mimimum and maximum cylinder, the medium is initially set to the background material (in this case air), followed by the assignment of the other materials to specific regions. A graphical representation of the example is shown on the front page of the manual using the `previewRZ` code discribed in the next section.

```
 ##########################
 :start geometrical inputs:

 METHOD OF INPUT= individual
 Z OF FRONT FACE= 0
 DEPTH BOUNDARIES=  0.00508, 0.2,
                    0.2011382,
                    0.3,
                    0.34,
                    0.41,
                    0.5,
                    0.51,
                    0.99,
                    1.0,
                    1.16,
                    1.96,
                    3.2,
                    3.5
 RADII=    0.025, 0.4, 0.45, 0.64, 0.85, 0.94, 1.18, 1.28, 1.5

 ######## Material Input
 MEDIA= GE512HPGE,          # 1
        AL512HPGE,          # 2
        TEF512HPGE,         # 3
        BE512HPGE,          # 4
        AIR512HPGE,         # 5
        MYLAR512HPGE,       # 6
        CU512HPGE,          # 7
        DELRIN512HPGE,      # 8
```

```
DESCRIPTION BY= planes
MEDNUM=        5, 4,  2,  6,  2,  2,  2,  8,  7,  2,  1,  3,  3
START ZSLAB=   1, 1,  1,  3,  3, 12, 12, 12, 11,  5,  8,  6,  7
STOP ZSLAB=   14, 1, 13,  3, 12, 13, 12, 13, 11, 10, 10,  6, 10
START RING=  1, 1,  8,  1,  6,  4,  5,  1,  1,  3,  1,  3,  5
STOP RING=   9, 8,  8,  6,  6,  4,  5,  3,  1,  5,  3,  5,  5

:stop geometrical inputs:
#########################
```

### 2.5.3 previewRZ

The utility `previewRZ` allows one to visualize the geometry and material data entered. It is a Tcl WISH (Simple windowing shell) script that parses the geometry and material input from your inputfile and draws a 2D graph with lines delimiting the regions of the RZ geometry specified in a given input file. The drawing is to scale. Regions are then filled with materials with colors assigned to each material.

Note that the location of the `wish` software (given in the first line of the script) needs to apply for your local system. For example, for the SUSE. distribution of Linux, the first line of the previewRZ program needs to be changed to `#!/usr/X11/bin/wish`. The command `which wish` will tell you the local location of `wish`.

The following is taken from the User Manual for the GUI's for the BEAM system[6].

> "All of the GUIs use `Tcl/Tk` and `wish`, a freeware package. The GUIs were developed using `Tcl` version 7.5, `Tk` version 4.1 and `wish` 4.1 or `wishx`. You can obtain version 8.4 of `Tcl/Tk` at `http://www.scriptics.com/software/8.4.html` or `http://www.activestate.com/Products/ActiveTcl`. We recommend using the the "ActiveTcl" site, since it includes a wizard which makes installation much easier (especially on Windows systems). Once you have installed `Tcl/Tk` you must ensure that the directory `/(directory where Tcl/Tk was installed)/bin` is included in your `PATH` environment variable. "

`previewRZ` can be invoked as follows (requires an alias defined in `egsnrc_cshrc_additions` for C-shells or `egsnrc_bashrc_additions` for Bourne shells if you are running on Unix/Linux):

```
previewRZ file
```

where `file` represents the `egsinp` file with or without extension. `previewRZ` can also be invoked from the `egs_inprz` GUI[5].

An example of previewing the geometry defined in previous section is shown on the cover of this manual.

The button `Plot Properties` allows one to adjust the limits of the viewing window. It is useful if, for example, the maximum limits of the geometry are much further away than the spacing between all other planes and cylinders. The button `Print` allows printing the geometry or saving it in a postscript file format. Settings in the `Print` box are self-explanatory.

### 2.5.4 preview3d

The EGS_Windows system for 3-D displays of EGS geometries and histories[4] includes a utility code called `preview3d.tcl` which also reads the input files for the RZ codes but in this case prepares an `.egsgeom` file for input to EGS_Windows. This allows a 3-D display of the geometry in combination with the tracks of the histories which can be obtained with any of these user codes using the `IWATCH` input for `SUBROUTINE WATCH` (see section 2.9.1).

## 2.6 Monte Carlo transport parameter control

All EGSnrc user codes, including the NRC RZ codes, require the setting of the Monte Carlo transport parameters. Since this is common to all codes, the inputs for the Monte Carlo transport parameter controls are gathered in the routine `get_transport_parameter(ounit)` where `ounit` represents the output unit (usually 6). The routine is located in the file `$HEN_HOUSE/get_inputs.mortran` and can be used by any user code.

The routine `get_transport_parameter(ounit)` will set all the variables that control the transport. In the inputfile, a section delimited by `:start mc transport parameter:` and `:stop mc transport parameter:` is required to input the parameters. But all input associated with selection of various transport parameter is not crucial for the execution as there are default values set. Therefore, if some of the input options in this section are missing/misspelled, this will be ignored and default parameter assumed. However, as the transport parameter input routine uses `GET_INPUT`, a lot of error/warning messages may be produced on UNIT 15. If you don't have the intention of changing default settings, simply ignore the error messages. So, for example, most of the tutorial codes do not input these variables since they are not changed from their defaults.

Note that the defaults are mostly those of EGSnrc. The defaults may often only add time to your calculation, and you can speed things up by turning them off (e.g. the photo-electron angular sampling, or relaxation in electron or high-energy photon beams) or bound Compton interactions vs Klein-Nishina scattering.

Currently, the following options are available (case does not matter except for the different cross-section compilations inputs and the internal variables are shown in [ ] brackets). Note that the default mentioned is the default for EGSnrc. These are NOT always the defaults used in the example/template input files)

```
Global ECUT=     Global (in all regions) electron transport cut
                 off energy (in MeV). If this imput is missing,
                 AE(medium) will be used.
                 [ ECUT ]

Global PCUT=     Global (in all regions) photon transport cut
                 off energy (in MeV). If this imput is missing,
                 AP(medium) will be used.
                 [ PCUT ]

Global SMAX=     Global (in all regions) maximum step-size
```

```
                restriction for electron transport (in cm).
                If missing, no geometrical step-size restrictions
                will be employed. Note that if you use the default
                EGSnrc electron-step algorithm, no SMAX-restriction
                is necessary. Option is useful for transport in low
                density materials (air) when PRESTA behaviour is
                turned on (see below)
                [ SMAXIR ]

ESTEPE=         Maximum fractional energy loss per step.
                Note that this is a global option only, no
                region-by-region setting is possible. If missing,
                the defualt is 0.25 (25%).
                [ ESTEPE ]

XImax=          Maximum first elastic scattering moment per step.
                Default is 0.5, NEVER use value greater than 1 as
                this is beyond the range of MS data available.
                [ XIMAX ]

Boundary crossing algorithm=
                There are two selections possible: EXACT, means
                the algorithm will cross boundaries in a single
                scattering (SS) mode, the distance from a boundary
                at which the transition to SS mode is made is
                determined by 'Skin depth for BCA' (see below).
                The second option is PRESTA-I, if selected boundaries
                will be crossed a la PRESTA, i.e. with lateral
                correlations turned off and MS forced at boundaries.
                Default is EXACT.
                [ bca_algorithm, exact_bca ]

Skin depth for BCA=
                Determines the distance from a boundary (in elastic
                MFP) at which the algorithm will go into single
                scattering mode (if EXACT boundary crossing) or
                swith off lateral correlations (if PRESTA-I boundary
                crossing). Default value is 3 for EXACT or
                exp(BLCMIN)/BLCMIN for PRESTA-I (see the PRESTA paper
                for a definition of BLCMIN). Note that if you choose
                EXACT boundary crossing and set Skin depth for BCA
                to a very large number (e.g. 1e10), the entire
                calculation will be in SS mode. If you choose
                PRESTA-I boundary crossing and make Skin depth for BCA
                large, you will get default EGS4 behavious (no PRESTA)
                [ skindepth_for_bca ]

Electron-step algorithm=
```

```
                PRESTA-II (the default), the name is
                used for historical reasons
                or PRESTA-I
                Determines the algorithm used to take into account
                lateral and longitudinal correlations in a
                condensed history step.
                [ transport_algorithm ]

Spin effects=   Off, On, default is On
                Turns off/on spin effects for electron elastic
                scattering. Spin On is ABSOLUTELY necessary for
                good backscattering calculations. Will make a
                difference even in 'well conditioned' situations
                (e.g. depth dose curves for RTP energy range
                electrons).
                [ spin_effects ]

Brems angular sampling= Simple, KM, default is KM
                If Simple, use only the leading term of the Koch-Motz
                distribution to determine the emission angle of
                bremsstrahlung photons. If On, complete
                modified Koch-Motz 2BS is used (modifications
                concern proper handling of kinematics at low energies,
                makes 2BS almost the same as 2BN at low energies).
                [ IBRDST ]

Brems cross sections= BH, NIST, NRC default is BH
                If BH is selected, the Bethe-Heitler bremsstrahlung
                cross sections (Coulomb corrected above 50 MeV)
                will be used. If NIST is selected, the NIST brems
                cross section data base (which is the basis for
                the ICRU radiative stopping powers) will be employed.
                Differences are negligible for E > ,say, 10 MeV,
                but significant in the keV energy range. If NRC is
                selected, the NRC brems cross-section data base will
                be used, which is a version of the NIST data base
                with corrected electron-electron brems contributions
                (corrections to the NIST data is typically only
                significant for low values of the atomic number Z
                and for k/T < 0.005).
                [ ibr_nist ]

Triplet production= On or Off (default).  Turns on/off simulation
                of triplet production.  If On, then Borsellino's
                first Born approximation is used to sample triplet
                events based on the triplet cross-section data.
                [ itriplet ]
```

```
Bound Compton scattering=  On, Off, Simple or norej (default)
                If Off, Compton scattering will be treated with
                Klein-Nishina, with On Compton scattering is
                treated in the Impulse approximation.
                With Simple, the impulse approximation incoherent
                scattering function will be used (i.e., no Doppler
                broadenning). With norej the actual total bound
                Compton cross section is used and there are no
                rejections at run time.
                Make sure to turn on for low energy applications,
                not necessary above, say, 1 MeV.
                [ IBCMP ]

Radiative Compton corrections= On or Off (default). If on, then
                include radiative corrections for Compton scattering.
                Equations are based on original Brown & Feynman
                equations (Phys. Rev. 85, p 231--1952).  Requires
                a change to the user codes Makefile to include
                $(EGS_SOURCEDIR)rad_compton1.mortran in the
                SOURCES (just before
                $(EGS_SOURCEDIR)get_inputs.mortran).
                [ radc_flag ]

Electron Impact Ionization= Off (default), On, casnati, kolbenstvedt,
                gryzinski or penelope.  If set to On or ik, then
                use Kawrakow's theory to derive EII cross-sections.
                If set to casnati, then use the cross-sections of
                Casnati (from file $HEN_HOUSE/data/eii_casnati.data).
                Similar for kolbenstvedt, gryzinski and penelope.
                This is only of interest in kV X-ray calculations.
                Note that the user can supply their own EII
                cross-section data as well. The requirement is that
                the file eii_suffix.data exists in the $HEN_HOUSE/data
                directory, where suffix is the name specified.
                Entry is case-sensitive except for Off, On or ik.
                [ eii_flag, eii_xfile ]

Pair angular sampling= Off, Simple, KM.
                If off, pairs are set in motion at an angle m/E
                relative to the photon direction (m is electron rest
                energy, E the photon energy). Simple turns on
                the leading term of the angular distribution
                (this is sufficient for most applications),
                KM (comes from Koch and Motz) turns on using 2BS
                from the article by Koch and Motz.  Uniform
                Default is Simple, make sure you always use
                Simple or KM
                [ IPRDST ]
```

```
Pair cross sections= BH (default) or NRC.  If set to BH, then use
                Bethe-Heitler pair production cross-sections.  If set
                to NRC, then use NRC pair production cross-sections
                (in file $HEN_HOUSE/data/pair_nrc1.data).  Only
                of interest at low energies, where the NRC cross-
                sections take into account the assymmetry in the
                positron-electron energy distribution.
                [ pair_nrc ]

Photon cross sections= Photon cross-section data.  Current options are
                si (Storm-Israel--the default), epdl (Evaluated Photon
                Data Library), xcom, and pegs4.  Allows the use of photon
                cross-sections other than from the PEGS4 file unless
                the pegs4 option is specified.
                Note that the user can supply their own cross-section
                data as well.  The requirement is that the files
                photon_xsections_photo.data,
                photon_xsections_pair.data,
                photon_xsections_triplet.data, and
                photon_xsections_rayleigh.data exist in the
                $HEN_HOUSE/data directory, where photon_xsections
                is the name specified.
                Entry is case-sensitive except for the pegs4 option.
                [ photon_xsections ]

Photon cross-sections output= Off (default) or On.  If On, then
                a file $EGS_HOME/user_code/inputfile.xsections is
                output containing photon cross-section data used.
                [ xsec_out ]

Compton cross sections= Bound Compton cross-section data.  User-
                supplied bound Compton cross-sections in the file
                $HEN_HOUSE/data/comp_xsections_compton.data, where
                comp_xsections is the name supplied for this input.
                This is only used if Bound Compton scattering= Simple
                and is not available on a region-by-region basis
                (see below).  The default file (ie in the absence
                of any user-supplied data) is compton_sigma.data.
                [ comp_xsections ]

Rayleigh scattering= Off, On, custom
                If On, turned on coherent (Rayleigh) scattering.
                Default is Off. Should be turned on for low energy
                applications. If custom, user must provide media names
                and form factor files for each desired medium. The
                rest of the media use the default atomic form factors.
                Not set to On by default for historical reasons since
```

```
                a PEGS4 data set is not required anymore.
                [ IRAYLR ]

ff media names = A list of media names (must match media found in
                PEGS4 data file) for which the user is going to
                provide custom Rayleigh form factor data.
                [ iray_ff_media($MXMED) ]

ff file names = A list of names of files containing the Rayleigh
               form factor data for the media specified by
               the ff media names = input above.  Full directory
               paths must be given for all files, and for each medium
               specified, iray_ff_media(i), there must be a
               corresponding file name, iray_ff_file(i).  For
               example files, see the directory
               $HEN_HOUSE/data/molecular_form_factors.
               [ iray_ff_file($MXMED) ]

Photoelectron angular sampling= Off or On
                If Off, photo-electrons get the direction of the
                'mother' photon, with On, Sauter's furmula is
                used (which is, striktly speaking, valid only for
                K-shell photo-absorption).
                If the user has a better approach, replace the macro
                    $SELECT-PHOTOELECTRON-DIRECTION;
                The only application that
                I encountered until now where this option made a
                small difference was a big ion chamber (cavity size
                comparable with electron range) with high-Z walls
                in a low energy photon beam.
                Default is On
                [ IPHTER ]

Atomic relaxations= Off, On
                Default is On. The effect of using On is twofold:
                - In photo-electric absorption events, the element
                  (if material is mixture) and the shell the photon
                  is interacting with are sampled from the appropriate
                  cross seections
                - Shell vacancies created in photo-absorption events
                  are relaxed via emission of fluorescent X-Rays,
                  Auger and Koster-Cronig electrons.
                 Make sure to turn this option on for low energy
                 applications.
                 [ IEDGFL ]
```

Atomic relaxations, Rayleigh scattering, Photoelectron angular sampling and Bound Compton scattering can also be turned On/Off on a region-by-region basis. An example for Atomic

relaxations on a region- by-region basis is:

```
Atomic relaxations= On in Regions   or
Atomic relaxations= Off in regions
```

Then define the regions in which you want the feature to be turned on:

```
Bound Compton start region=
Bound Compton stop region=
         or
Rayleigh start region=
Rayleigh stop region=
         or
Relaxations start region=
Relaxations stop region=
         or
PE sampling start region=
PE sampling stop region=
```

each followed by a list of one or more start and stop regions separated by commas. Example:

```
Atomic relaxations= On in Regions
Relaxations start region=  1, 40
Relaxations stop region=  10, 99
```

will first turn off relaxations everywhere and then turn on in regions 1-10 and 40-99. Note that the input is checked against minimum and maximum region number and ignored if `start region < 1` or `stop_region > $MXREG` or `start region > stop region`.

`ECUT`, `PCUT` and `SMAX` can also be set on a region-by-region basis. To do so, include in the input file

```
Set XXXX=              f_value1, f_value2, ...
Set XXXX start region= i_value1, i_value2, ...
Set XXXX stop region=  j_value1, j_value2, ...
```

where `XXXX` is `ECUT`, `PCUT` or `SMAX`, `f_value1`, `f_value2`,... are the desired values for `XXXX` and `i_value_i` and `j_value_i` are the start and stop regions.

## 2.7 Source and energy distribution routine inputs

The RZ codes systematically make use of the same source routines. These routines are located in the files `srzrc.mortran` and `ensrc.mortran` which are concatenated with the RZ code in the process of producing the overall source code file as specified in the `user_code.make` file (see section 2.18). Input of the type of source and the source parameters are defined within the delimiters `:start source inputs:` and `:stop source inputs:`.

For all source types discussed below the parameters `INCIDENT PARTICLE` and `SOURCE NUMBER` need to be assigned to set the charge of the incident beam and the source number respectively.

```
  INCIDENT PARTICLE=  electron   (-1)  electrons
                      photon     (0)   photons
                      positron   (1)   positrons
(for SOURCE 21,22,23) all        (2)   include all of the particles
                                       in the phase space file
                                       [IQIN]
  SOURCE NUMBER=                 (I)   number of the source
                                       [ISOURC]
```

The currently implemented source numbers are: 0, 1, 2, 3, 4, 10, 11, 12, 13, 14, 15, 16, 20, 21, 22 and 23. Table 1 describes the sources and the required input to be assigned to the string `SOURCE OPTIONS=`. The values need to be input, even if all zeros. Some sources have inputs in addition to those on the `SOURCE OPTIONS=` line. These are also indicated in the table.

Note that point and extended sources off axis (source 12, 15, 16) use sampling algorithms that make the calculation inefficient because of strongly varying weights if the source is close to the geometry ("close" or "far" is to be understood as a comparison between source to geometry distance and geometry size, *i.e.* a point source that is 3 cm away from a geometry 0.5 cm across is "far" and a point source 100 cm away from a 200 cm geometry is "close"). Note also that source 16 (extended source off axis) can be made equivalent to source 12 and 15, which are two different implementations of a point source off axis.

Table 1: Description of the `SOURCE OPTIONS=` inputs for the source routines in the RZ codes. Additional inputs are also indicated where required. Delimeters are: `:start source inputs:` and `:stop source inputs:`.

| Source Number | Parameters | Description |
|---|---|---|
| 0 | | **Parallel beam incident from front (+Z-axis)** |
| | | RBEAM, UINC, VINC, WINC |
| | RBEAM | radius of parallel beam in cm |
| | | (defaults to the max radius of geometry) |
| | UINC,VINC,WINC | incident x,y,z-axis direction cosines |

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| Source Number | Parameters | Description |
|---|---|---|
| | | Note: (UINC,VINC,WINC) get automatically normalized defaults to (0.0,0.0,1.0) |
| 1 | | **Point source on axis incident from front** |
| | | DISTZ, RBEAM, 0, 0 |
| | DISTZ | distance of the point source from the front of the target in cm (DEFAULT 100.) |
| | RBEAM | radius of the beam at the front of the target in cm (defaults to MAX radius) |
| 2 | | **Broad parallel beam from front (+Z-axis)** |
| | | Basically a one dimensional calculation. |
| | | 0, 0, 0, 0 |
| | | No input parameters needed. |
| 3 | | **Internal uniform isotropically radiating disk of finite size** |
| | | RMINBM, RBEAM, ZSMIN, ZSMAX |
| | RMINBM | inner radius of source region (inside overall geometry) |
| | RBEAM | outer radius of source region (inside overall geometry) |
| | ZSMIN | minimum z-coordinate of source |
| | ZSMAX | maximum z-coordinate of source |
| 4 | | **Central axis depth-dose vs. beam radius** |
| | | RCAXIS, 0, 0, 0 |
| | RCAXIS | radius of central axis scoring zone (cm) Radii of scoring zones will be treated as beam radii. |
| 10 | | **Parallel beam incident from the side (along +Y-axis)** |
| | | XBEAM, ZBEAM, 0, 0 |
| | XBEAM | half-width of the rectangular beam in cm (defaults to max radius) |
| | ZBEAM | half-height of the rectangular beam in cm (defaults to max) |
| 11 | | **Point source incident from the side** |
| | | DISTRH, XBEAM, ZBEAM, 0 |
| | DISTRH | distance of the source from the middle of the target in cm (defaults to 100.) |
| | XBEAM | half-width of the beam at the center of the target in cm (defaults to max radius) |
| | ZBEAM | half-height of the beam at the center of the target in cm (defaults to max) |
| 12 | | **Point source off axis** |

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| Source Number | Parameters | Description |
|---|---|---|
| | | DISTRH, DISTZ, 0, 0 |
| | DISTRH | distance of the point source off the Z-axis |
| | DISTZ | perpendicular distance of the point source from the front face<br>if `DISTZ`>0<br>point is located in front of front face<br>if 0 > `DISTZ` > `-(ZPLANE(NPLANE)-ZPLANE(1))`<br>point located between front and rear face<br>`DISTZ` < `-(ZPLANE(NPLANE)-ZPLANE(1))`<br>point located rear of rear plane |
| 13 | | **Parallel beam from any angle** |
| | | UINC, VINC, WINC, 0 |
| | UINC | incident x-axis direction cosine |
| | VINC | incident y-axis direction cosine |
| | WINC | incident z-axis direction cosine<br>Note: (UINC,VINC,WINC) get automatically normalized. Default is (0.0,0.0,1.0) |
| 14 | | **Point source on axis incident from the front with all events inside RMINBM not followed** |
| | | DISTZ, RBEAM, RMINBM, 0 |
| | DISTZ | distance of the point source from the front of the target in cm (defaults to 100.) |
| | RBEAM | radius of the beam at the front of the target in cm (defaults to max radius) |
| | RMINBM | below this radius, all histories are terminated by the source routines by giving them zero weight. The HOWFAR routines must check for this. |
| 15 | | **Point source incident from any angle** |
| | | DIST, ANGLE, 0, 0 |
| | DIST | distance from the centre of the geometry to the point source (cm) |
| | ANGLE | angle of rotation around the axis that is parallel to the x axis and passes trough the centre of the geometry (degrees).<br>0 degrees corresponds to source above front face of geometry.<br>Note: The point source must be outside the geometry. |
| 16 | | **Circular or rectangular isotropically-radiating source from any angle** |
| | | DIST, ANGLE, TMP1, TMP2 |
| | DIST | distance from the centre of the geometry to the |

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| Source Number | Parameters | Description |
|---|---|---|
| | | centre of the source plane (cm) |
| | ANGLE | angle of rotation of source plane around the axis that is parallel to the x axis and passes trough the centre of the geometry (degrees). Zero degrees corresponds to the source incident on the front face of the geometry. |
| | TMP1 | if $> 0$ and TMP2 $\leq 0$: TMP1 = radius of source (cm)<br>if $\geq 0$ and TMP2 $\geq 0$: TMP1 = half-width of source in x direction (cm) |
| | TMP2 | if $> 0$ and TMP1 $\leq 0$: TMP2 = radius of source (cm)<br>if $\geq 0$ and TMP1 $\geq 0$: TMP2 = half-width of source in y direction (cm)<br>Note: if TMP1 $\leq 0$ and TMP2 $\leq 0$, then this becomes a point source incident from any angle, identical to source 12 and 15. |
| 17 | **Point source on-axis incident from the front (square collimation)** | |
| | | DISTZ, XBEAM, YBEAM, 0 |
| | DISTZ | distance of source from front of geometry (cm). Defaults to 100 cm. |
| | XBEAM | half-width in X-direction at front of geometry (cm). |
| | YBEAM | half-width in Y-direction at front of geometry (cm). |
| 20 | **Radial distribution input** | |
| | This source has no SOURCE PARAMETERS= inputs | |
| | **Additional inputs:** | |
| | MODEIN= Local | if radial distribution is to be input as part of the .egsinp file |
| | MODEIN= External | if the distribution is to be input via an external file |
| | if MODEIN = Local | |
| | NRDIST | Number of radial bins in distribution histogram |
| | RDISTF | top of radial bin should be NRDIST values |
| | RPDF | Probability of initial particle being in this bin. Probability doesn't need to be normalized but it should be in units $cm^{-2}$ Should be values for 1 to NRDIST. |
| | RDIST IOUTSP= None | No distribution data in output summary |
| | = Include | include distribution data output summary |
| | if MODEIN = External | RDIST FILENAME |
| | RDIST FILENAME | filename(with ext) contains distribution info |

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| Source Number | Parameters | Description |
|---|---|---|
| | | in the same format as described above. |
| | RDIST IOUTSP | See above |
| 21 | | **Full beam phase space data, incident on front face** |
| | | IMODE, NRCYCL, IPARALLEL, PARNUM |
| | IMODE | set to 0 for 7 variables/record: X,Y,U,V,E,WT,LATCH<br>set to 2 for 8 variables/record: the above + ZLAST |
| | NRCYCL | no. of times to reuse each particle before moving on to the next one. Thus, each particle is used a total of NRCYCL+1 times. Use of NRCYCL is essential for accurate statistics when NCASE > no. of particles in the phase space file. If set ≤0, then NRCYCL is automatically calculated to use the entire phase space file with no restarts based on NCASE, incident particle type, and the number of particles with the appropriate charge in the phase space file. Note that the automatic calculation of NRCYCL is not done if INCIDENT PARTICLE= positron. Also, the automatically-calculated value of NRCYCL does not take into account particles rejected because they miss the geometry or because they have crossed the phase space plane multiple times. |
| | IPARALLEL | set >1 if you are splitting the simulation into IPARALLEL jobs. IPARALLEL is used with PARNUM (see below) to partition a phase space source into IPARALLEL equal parts. |
| | PARNUM | For each of the IPARALLEL parallel jobs, PARNUM should have a different integer value in the range<br>range 1≥PARNUM≤PARALLEL. The partition of the phase space source that is used for a job is then given by:<br>(PARNUM-1)*(NCASE_PHSP/IPARALLEL)<NPHSPN≤<br>(PARNUM)*(NCASE_PHSP/IPARALLEL)<br>where NCASE_PHSP is the total number of particles in the phsp source and NPHSPN is the particle no. chosen. Note that use of IPARALLEL and PARNUM is not necessary if you are |

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| Source Number | Parameters | Description |
|---|---|---|
| | | using the built-in parallel processing functionality of these codes. |
| | Note: IPARALLEL and PARNUM are not used with the built-in EGSnrc_MP parallel processing functionality. | |
| | **Additional inputs:** | |
| | FILSPC= | Filename (with ext) containing the phase space info (max. 80 characters) assigned to unit 42. |
| 22 | **Full beam phase space data, incident from any angle/position** | |
| | IMODE, DIST, ANGLE, ZOFFSET, NRCYCL, IPARALLEL, PARNUM, XOFFSET, YOFFSET | |
| | IMODE | set to 0 for 7 variables/record: X,Y,U,V,E,WT,LATCH<br>set to 2 for 8 variables/record: the above + ZLAST |
| | DIST | distance from source plane to the point (x,y,z)=(0,0,ZOFFSET) in cm. Defined so that, when ANGLE=0, DIST is in the -z direction. |
| | ANGLE | angle of rotation about the Z axis (degrees). ANGLE = 0 means particles are incident in the +ve z direction. |
| | ZOFFSET | defines the z offset of point from which DIST is measured. If \|ZOFFSET\| > 1e4, then it defaults to the centre of the geometry. |
| | NRCYCL | See source 21 above. |
| | IPARALLEL | See source 21 above. |
| | PARNUM | See source 21 above. |
| | XOFFSET | X offset of source plane. |
| | YOFFSET | Y offset of source plane. X and Y offsets are applied before any rotations by ANGLE. |
| | **Additional inputs:** | |
| | FILSPC= | Filename (with ext) containing the phase space info (max. 80 characters) assigned to unit 42. |
| 23 | **Full BEAM simulation, incident from any angle/position** | |
| | DIST, ANGLE, ZOFFSET, XOFFSET, YOFFSET | |
| | DIST | See source 22 above. Note that the source plane is the phase space scoring plane in the BEAM simulation being used as a source. See below for more details. |
| | ANGLE | See source 22 above. |
| | ZOFFSET | See source 22 above. |
| | XOFFSET | See source 22 above. |
| | YOFFSET | See source 22 above. |
| | **Additional inputs:** | |
| | BEAM CODE= | The name of the BEAM accelerator code |

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| Source Number | Parameters | Description |
|---|---|---|
| | | being used as a source, including the `BEAM_` prefix (i.e. `BEAM_accelname`). This code must have been compiled as a shared library (see the BEAMnrc manual for information on how to do this) and exist as `BEAM_accelname.so` (for Linux/Unix) or `libBEAM_accelname.dll` (for Windows) in your `$EGS_HOME/bin/config` directory. |
| | INPUT FILE= | The name of the input file used for the accelerator (no `.egsinp` extension). This file must exist in your `$EGS_HOME/BEAM_accelname` directory and must specify output of a phase space file at one scoring plane. Instead of being written to a phase space file, particles are extracted and used as source particles upon crossing this plane. |
| | PEGS FILE= | The name of the pegs4 data set to be used in the BEAM simulation (no `.pegs4dat` extension). The pegs4 data must exist in `$HEN_HOUSE/pegs4/data` or in your `$EGS_HOME/pegs4/data` directory. |
| | WEIGHT WINDOW= | Set to MIN_WEIGHT_23, MAX_WEIGHT_23, where MIN_WEIGHT_23 = min. weight of source particles to use (defaults to -1E30) and MAX_WEIGHT_23 = max. weight of source particles to use (defaults to 1E30). |
| | Note that the Z-position of the scoring plane, where incident particle data is collected, in the BEAM simulation is not passed to the RZ code. Thus, similar to a phase space source, the incident position of the source plane, defined by `DIST`, `ANGLE`, `ZOFFSET`, `XOFFSET` and `YOFFSET`, is independent of the BEAM coordinate system. | |

Particles can be sampled from energy distributions, but this is independent of the geometric source routines. For SOURCE=21,22,23 each individual particle is taken from a phase space file or BEAM simulation, and sampling from an energy distribution is not required. To sample from an energy distribution specify the following variables within the delimiters `:start source inputs:` and `:stop source inputs:`:

```
INCIDENT ENERGY=   monoenergetic       if monoenergetic beam
                   spectrum            if energy spectrum to be used
         ---------------------------------------
If INCIDENT ENERGY= Monoenergetic:
   INCIDENT KINETIC ENERGY(MEV)=   kinetic energy of the incident
                                   beam in MeV (defaults to 1.25)
         ---------------------------------------
```

```
If INCIDENT ENERGY= Spectrum:
         SPEC FILENAME   (C)filename (with ext)
                            contains spectral information
                            FILE FORMAT:
                            TITLE      spectrum title  (80 char)
                            NENSRC, ENMIN, MODE (on 1 line)
                              NENSRC     # energy bins in spec. histogram
                              ENMIN      lower energy of first bin
                              MODE       =0, assumes cts/bin
                                         =1  assumes cts/MeV
                            ENSRCD(I),SRCPDF(I)  I=1,NENSRC pair/line
                            top of energy bin and probability of
                            initial particle being in this bin.
                            probability does not need to be normalised
        SPEC IOUTSP
            = none          no spectrum in output summary
            = include       include spectrum in output summary
```

## 2.8 Common Variance Reduction Inputs

Three variance reduction techniques have been incorporated in EGSnrc rather than left to the user codes, *i.e.*,

- Electron range rejection
- Bremsstrahlung splitting
- Russian Roulette

Further in this section we briefly outline what the techniques mean, and then go on to explain the inputs. In the RZ user codes, two additional techniques are implemented:

- Pathlength biasing
- Photon Forcing

We will also deal with these techniques in this section. The delimiters for these inputs are `:start variance reduction:` and `:stop variance reduction:`.

Additional variance reduction techniques are available in DOSRZnrc (photon cross section enhancement) and CAVRZnrc (photon cross section enhancement and photon splitting). These will be discussed in the portions of the manual related to these codes.

### 2.8.1 Electron Range Rejection

Range rejection has been discussed in the EGSnrc Manual [7] in section 3.9.1 and is a valuable tool to save cpu time. Briefly it allows the user to terminate the history of an

electron when it's residual CSDA range is such that it cannot possibly reach another region and deposit energy in that region. However, by terminating the history, the possibility of a bremsstrahlung photon being created and escaping from the region is eliminated. To control this approximation an energy threshold is defined, `ESAVEIN`, (formerly `ESAVE`), above which no range rejection is done. An intelligent choice of this energy must depend on Z and is essentially made based on knowing the approximate fraction lost to bremsstrahlung in a specific material. The inputs for range rejection are as follows.

```
ELECTRON RANGE REJECTION
       = off        (0)  No electron range rejection
       = on         (1)  Do electron range rejection. All charged
                         particles without enough range to get out
                         of their current region have their
                         history terminated.  This uses EGSnrc internal
                         range rejection and takes no time to test.
                         The parameter ESAVEIN also plays a role (see below)
                         [IREJCT]

ESAVEIN             (R)  If ELECTRON RANGE REJECTION is on, discard an
                         electron  when E< ESAVEIN and RANGE < distance
                         to the nearest boundary.
                         This ignores bremsstrahlung losses below ESAVEIN.
                         This parameter must be input even if not used.
                         ESAVEIN is a total energy.
```

`ESAVEIN` gets assigned to `e_max_rr(irl)` for all regions present in the simulation.

In the previous versions of DOSRZ and CAVRZ there was another range rejection capability wherein the user specified a region of interest and a parameterisation of the range for charged particles in all regions outside the region of interest. Range rejection was performed on all particles which could not reach the region of interest given the range function. This could be very useful, especially for homogeneous phantoms. This has not yet been implemented in DOSRZnrc but CAVRZnrc has an additional form of range rejection which is automatically turned on whenever range rejection is on. Basically it defines the region of interest as the smallest cylinder which completely encompasses any region made of the same material as the cavity region (assuming it is a gas and therefore having a long range). An automatic search is made of all materials outside this cylinder and the material with the longest range is used for applying the range rejection to the cylinder of interest. In many, but not all cases, this form of range rejection can be very efficient.

### 2.8.2 Bremsstrahlung splitting and Russian Roulette

Bremsstrahlung splitting can be a very powerful technique if the user is interested in brem beams. In accelerator modelling it has been shown that splitting factors of 20 – 40 are optimal[3] and can save a factor of 4 in computing time.

```
BREM SPLITTING
       = Off            (0)   no bremsstrahlung splitting
```

```
       = On             (1)   there is bremsstrahlung splitting

 NUMBER OF BREMS PER EVENT
                        (I)   number of brems / event if splitting on

 CHARGED PARTICLE RUSSIAN ROULETTE
       = Off        (0)  No Russian Roulette with charged particles
       = On         (1)  Play Russian Roulette with charged particles with
                         probability of survival=PROB_RR=1/nbr_split.
                         [I_PLAY_RR]
```

The above form of Russian Roulette is meant to complement the use of bremsstrahlung splitting for those cases where only the photons are of significant interest. It is designed to ensure that charged particles carry their natural weight. It is implemented using the internal EGSnrc option.

Most user codes (CAVRZnrc, DOSRZnrc, SPRRZnrc, CAVSPHnrc) also have a photon Russian Roulette option which is set using the inputs:

```
 RUSSIAN ROULETTE DEPTH      (R)
                      for Russian roulette - as any photon
                      crosses the Z='RUSSIAN ROULETTE DEPTH'
                      plane,  Russian roulette is played.
                      [RRZ]

 RUSSIAN ROULETTE FRACTION   (R)
                      Each time Russian roulette is played, RRF
                      is the probability of survival.
                      weight increases by 1/RRF,  if it survives
                      [RRCUT]

              ****** IF BOTH ZERO, NO RUSSIAN ROULETTE IS PLAYED ******
```

As indicated above, every time a photon is about to cross an imaginary plane at Z given by `RUSSIAN ROULETTE DEPTH`, Russian Roulette is played on that particle, and it survives with a probability given by `RUSSIAN ROULETTE FRACTION`. If the photon does survive, then its weight is increased by 1/`RUSSIAN ROULETTE FRACTION`.

### 2.8.3 Photon pathlength biasing (DOSRZnrc only)

Pathlength biasing is a technique to decrease or increase the path length of a photon in order to improve statistics in a specific region of interest. The technique of pathlength biasing by using an exponential transformation of photon path lengths is discussed in Ref [8]. Briefly, the distance to the next photon interaction is calculated from:

$$\eta = -\frac{1}{1 - C\cos\theta} lnR \tag{1}$$

where $C$ is a user-defined variable, $R$ a random number, and $\theta$ the angle between the direction of the photon and the direction of interest, (*e.g.*, the depth axis for a depth-dose curve). For $C < 0$ pathlengths are compressed, for $0 < C < 1$ pathlengths are stretched in the forward direction which may be suitable for specific applications. The scored quantities are weighed by multiplying each contribution with $\frac{e^{\eta C cos\theta}}{1-Ccos\theta}$ The method can be activated in DOSRZnrc by defining the $C$ parameter in the input as follows:

```
EXPONENTIAL TRANSFORM C=
                  Parameter for pathlength biasing
                  If < 0       ==> shortening of forward pathlengths
                  If 0 < C < 1 ==> stretching of forward pathlength
                  If 0.0       ==> no biasing done
                  [CEXPTR]
```

This techniques was first implemented to allow for more efficient studies of the dose buildup region in photon beams[9, 10] (with `C < 0.0`) but it would be equally useful in deep penetration problems (with `0 < C < 1`).

### 2.8.4 Photon forcing

Photon forcing is a technique to force an interaction within the geometry between the current point and the point where the photon exits the geometry. This method is described in detail in Ref. [8]. Briefly, the number of mean free paths (#MFP) to the next interaction is selected using:

$$\eta = -ln\left[1 - R(1 - e^{-X})\right] \tag{2}$$

where $X$ is the maximum #MFP the photon can travel in its current direction within the geometry. The maximum #MFP must be found by pre-tracking the photon through the geometry in its current direction and summing the #MFP along its straight path. In this case contributions to scored quantities are weighed by multiplying with $(1 - e^{-X})$. The method can be applied to as many generations of scattered photons as required.

This technique is almost essential for calculations involving very thin geometries and incident photons. It can also be very helpful if, e.g. one is studying the contribution of scattered photons in an ion chamber (as done in CAVRZnrc).

This method can be activated in the input file by specifying the following parameters.

```
PHOTON FORCING
      = Off          (0)    normal photon transport (no forcing)
      = On           (1)    force photon interactions explicitly
                            must set START and STOP FORCING in this case
                            [IFORCE]

START FORCING        (I)    number of photon interaction/history at which
                            to start forcing photon interactions
                            This input is required even if forcing off
                            [NFMIN]
```

```
STOP FORCING AFTER  (I)    number of photon interaction/history after which
                           to stop forcing photon interactions
                           [NFMAX]
                           STOP FORCING AFTER must be >= START FORCING
                           This input is required even if forcing off
```

## 2.9 Common I/O Control

I/O control inputs must be input between the delimiters `:start I/O control:` and `:stop I/O control:`. This section will describe those I/O controls that are common to all user codes. I/O controls specific to each user code are described in the separate user code sections below.

### 2.9.1 The WATCH outputs, including EGS_Windows

The NRC subroutine WATCH (located in the file `nrcaux.mortran`) allows the user to follow the physics of the simulation, and is very useful for debugging purposes. WATCH has already been discussed in relation to `tutor4.mortran` (see section 4.4 of the EGSnrc user manual[7]).

The following WATCH inputs are possible in the RZ user codes.

```
IWATCH= off            for normal output
      = interactions   output info on every discrete interaction
      = steps          output on every electron/photon step as well
      = deposited      output when energy is deposited as well
      = graph          outputs file for EGS_Windows graphics
                       [IWATCH]
```

There is a large amount of output associated with running the code using the WATCH option activated. Be sure to pipe the output in that case through `more` or run in batch mode with only a few histories (10 to start) since the amount of ***output can be very large***.

### 2.9.2 STORE INITIAL RANDOM NUMBERS

All user codes give the user the option of storing random numbers at the beginning of each history using the `STORE INITIAL RANDOM NUMBERS` input. Random numbers are stored in a `.egsrns` file. You can restart the simulation using these random numbers using one of the `IRESTART` options, described in section 2.9.3(page 36).

The options for `STORE INITIAL RANDOM NUMBERS` are:

```
STORE INITIAL RANDOM NUMBERS
      = no          (0)  do not store initial random numbers
      = last        (1)  store initial random number for last history
```

```
      = all          (2)  store all initial random numbers
```

If you set `STORE INITIAL RANDOM NUMBERS= last`, then, at the start of each history, the `.egsrns` will be overwritten with the random numbers for that history. Thus, at the end of the run, `.egsrns` will store the random numbers for the last history.

If you set `STORE INITIAL RANDOM NUMBERS= all`, then, instead of overwriting the previous random numbers in `.egsrns` at the start of each history, the random numbers for the current history will be appended to the random number data already in `.egsrns`. Thus `.egsrns` will contain a record of random numbers for all histories from the first to the last.

CAVRZnrc has an additional option, `STORE INITIAL RANDOM NUMBERS= all deposited`, which is not available for the other codes. See section 6.3(page 77) for more details.

Note that the `STORE INITIAL RANDOM NUMBERS` option is mostly used for debugging purposes.

### 2.9.3 IRESTART - restarting runs

All user codes offer several restart options. These are:

```
IRESTART
      = first        (0)  first run for this data set
      = restart      (1)  restart of a previous run
      = analyze      (3)  just read in the raw data and do the statistical
                          analysis
      = start-RNS    (4)  read starting random numbers from a file
      = parallel     (5)  Combine results from previous parallel runs
```

Set `IRESTART= first` if this is the first run of this simulation.

Use `IRESTART= restart` if you wish to take the data from this simulation and append it to the data from a previous run. If you use this option, your previous run must have been done with `STORE DATA ARRAYS= yes` (see section 2.9.4(page 37)). Note that CPU times are cumulative, so if you're restarting a run, then the maximum CPU time allowed (see section 2.10.3(page 39)) must account for the time of the previous run as well.

Use `IRESTART= analyze` if you have data from a previous run in a `.egsdat` file (you must have run it with `STORE DATA ARRAYS= yes`– see section 2.9.4(page 37)) and you want to reanalyze it and output the results to the `.egslst` file. This is very useful if you want to change the quantity that you are outputting from the data after you have already run the simulation.

When `IRESTART= start-RNS`, then your user code will use the random numbers stored in the `.egsrns` file (see section 2.9.2(page 35)) to run the simulation. If you ran the previous simulation with `STORE INITIAL RANDOM NUMBERS= last`, then the current simulation will run all histories with the same random numbers used by the last history in the previous run. In other words, all histories will be identical to this last history as long as nothing else has changed.

IRESTART= parallel is used to read the .egsdat files from separate parallel jobs, combine them, analyze them, and output the combined results to the .egslst file. See section 2.14(page 50) for more information on parallel runs. Note that this option assumes that the naming scheme for the .egsdat files from the parallel runs is:
inputfile_w(i).egsdat, inputfile_w(i+1).egdat,...
This is the naming scheme used by the pprocess script described in section 2.14(page 50). Note that the user code SPRRZnrc does not have the IRESTART= parallel option.

### 2.9.4 STORE DATA ARRAYS

The STORE DATA ARRAYS options are:

```
STORE DATA ARRAYS
      = yes             (0) Store data arrays for re-use
      = no              (1) don't store them
```

If you select STORE DATA ARRAYS= yes then, at the end of each output batch, the .egsdat file will be overwritten with:

1. the current random number state
2. the total number of histories so far (including restarts)
3. total fluence so far (including restarts) (not for all codes)
4. the total CPU time so far (including restarts)
5. the total number of particles read from a phase space source (including restarts)
6. the total number of charged particle steps taken (including restarts)
7. the total number of times multiple scattering has been switched off (including restarts)
8. Raw data needed by the code to calculate quantities of interest. These data are cumulative and include data from previous runs if this is a restart. Just the required sums are stored. The raw data stored will depend on the user code AND the output options requested by the user. For example, DOSRZnrc could store the total energy deposited in each region, the total-minus-stopper energy deposited in each region and (if STORE KERMA= yes), the kerma deposited in each region.

The .egsdat file is necessary for IRESTART= restart, IRESTART= analyze and IRESTART= parallel options described in Section 2.9.3(page 36). Note that the .egsdat file can become very large (we have seen 100 Mbyte), especially for the code FLURZnrc. For short runs, writing this file can dominate the simulation time and so it may be best not to store it, at least for any short runs or when large numbers of runs are being done in parallel.

## 2.10 Common Monte Carlo Inputs

The Monte Carlo inputs are delimited between `:start Monte Carlo inputs:` and `:stop Monte Carlo inputs:`. This section outlines those Monte Carlo input parameters which are common to all the user codes.

### 2.10.1 Number of Histories

In the NRC user codes, the variables related to the number of histories are all defined, by default, to be INTEGER*8 variables so that the maximum allowed value is of the order of $5\times10^{18}$, i.e. effectively infinite. However, not all compilers handle INTEGER*8. If your compiler is one of them (eg HP), you must change the definition of the macro `$LONG_INT`, which is defined in `egsnrc.macros`, from

```
REPLACE {$LONG_INT} WITH {;integer*8}
```

to

```
REPLACE {$LONG_INT} WITH {;integer*4}
```

In this case, the limit on the number of histories is 1,073,741,824 ($2^{30}$).

For `IWATCH` zero, the minimum number of histories is `$NBATCH`, the number of output batches. The default is 20,000 histories. If `IWATCH` is non-zero, there are no minimum number of histories, but the program will not complete properly if the number of histories is less than `$NBATCH`.

### 2.10.2 Random number seeds

The issue of random number initialisation and the generators provided with EGSnrc, viz RANLUX and RANMAR, are discussed at length in the EGSnrc Manual[7] (see sections 3.4.1.iv and 3.8). The NRC user codes have been written to allow use of both RNGs with the same input format, although with different meaning in each case. The default RNG is RANLUX. The inputs, which are always in the "`Monte Carlo inputs`" section of the input, are:

```
INITIAL RANDOM NO. SEEDS=  INTGER1, INTEGER2
           User-code can use RANLUX or RANMAR, depending on selection
           Default is RANLUX
     RANLUX
           INTEGER1 is the luxury level, use 1 to 4, 4 taking longest
                    default is 1 (set by $DEFAULT-LL in ranlux.macros)
           INTEGER2 selects the independent sequence to use, it
                    can be from 1 to 1073741824 (2**30)
     RANMAR
           INTEGER1 is a seed between 1 and 31328 (0 =>default 1802)
           INTEGER2 is a seed between 1 and 30081 (0 =>default 9937)
                    Selection of unique INTEGER2 values guarantees
```

```
                independent sequences.
Note:
      After the seeds are first input and used for initialization,
      the variables IXXIN and JXXIN are just pointers used by the RNG
```

### 2.10.3 Maximum CPU time

The user also enters the maximum CPU time allowed for the run in this section using the `MAX CPU HOURS ALLOWED` input. The default is `MAX CPU HOURS ALLOWED= 999.`, and the current maximum is 1000 hrs. This is the total CPU time for the run, including restarts. For parallel runs using EGSnrcMP's built-in parallel processing functionality (see section 2.14(page 50)), it is the maximum CPU time for each parallel job. At the end of each output batch, the amount of time required/batch is calculated and added to the total CPU time so far. If this is found to exceed `MAX CPU HOURS ALLOWED`, then the code exits with a message saying that there is not enough time for the next batch, and it will analyze the data that it has so far and output the results to the `.egslst` file.

Note that this input variable used to be important when jobs were killed arbitrarly at the end of a given time limit, but is not so useful in todays computing environment. Just set it to a large value or use the default of 999. h.

## 2.11 How statistics are handled

Prior to the 2002 release, the RZ user-codes used the batch method to estimate uncertainty on a scored quantity. At the end of the simulation, the average of each scored quantity, X (eg fluence in a voxel), was calculated over all batches, and the uncertainty on this average was given by:

$$s_{\overline{X}} = \sqrt{\frac{\sum_{i=1}^{N}(X_i - \overline{X})^2}{N(N-1)}} \tag{3}$$

where N was the number of batches, $X_i$ was the value of X in batch i and $\overline{X}$ was the mean value of X evaluated over all batches.

There are limitations to the batch method of estimating uncertainty. The small sample size, N, in Equation 3 means that there are large fluctuations in the uncertainty estimate. Also, the batch method ignores correlations between incident particles when a phase space or full BEAM simulation source is used (`ISOURC`=21, 22 or 23). Finally, the batch method, as implemented in these codes, used an extra dimension (storing batch number) to each scoring array. This may become a limitation if you are scoring in a huge number of voxels and/or using a large number of batches.

The batch method for estimating uncertainty has been phased out in favour of a history by history method which was first implemented in the BEAMnrc and DOSXYZnrc codes[11].

In the history by history method, we return to Equation 3, but now N is the number of primary (non-phase space) histories and $X_i$ is the contribution to X from primary history i.

The equation can be rewritten as:

$$s_{\overline{X}} = \sqrt{\frac{1}{N-1}\left(\frac{\sum_{i=1}^{N} X_i^2}{N} - \left(\frac{\sum_{i=1}^{N} X_i}{N}\right)^2\right)} \tag{4}$$

If we keep track of $\sum_{i=1}^{N} X_i^2$ and $\sum_{i=1}^{N} X_i$ on the fly, then we can calculate the uncertainty at the end of the simulation without the need to store the scored quantity in batches. Unfortunately, it can be very computationally inefficient to evaluate $\sum_{i=1}^{N} X_i^2$ at the end of each history. To overcome this problem, we use the following algorithm proposed by Sempau *et al.* [12] for quantity X:

```
IF(nhist=X_last) THEN
   X_tmp=X_tmp + delta
ELSE
   X=X+X_tmp
   X2=X2+(X_tmp)**2
   X_tmp=delta
   X_last=nhist
ENDIF
```

where `X` stores $\sum_{i=1}^{N} X_i$ during the run, but, after analysis, will store the quantity $\overline{X}$, `nhist` is the current history number, `X_last` is the last history that contributed to `X`, `X_tmp` stores the sum of the contributions to `X` during the current history, `delta` is a contribution to `X` during the current step, and `X2` stores $\sum_{i=1}^{N} X_i^2$.

The history by history method eliminates the three main problems with the batch method. Since N is now the number of primary histories, which is usually large for a calculation with reasonable statistics, the problem of small sample size is eliminated, and fluctuations in the uncertainty estimate are greatly reduced. Also, by grouping scored quantities according to primary (non-phase space) history, correlations between incident particles from a phase space source are taken into account because their contributions are included in the same primary history. Finally, we eliminate the extra dimension in scoring arrays required to store batch number in favour of a `REAL*8` array, `X2`, a `REAL*4` array, `X_tmp`, and a `INTEGER*8` array, `X_last`, for an overall decrease in memory requirement.

The RZ user-codes also output ratios of two scored quantities which are correlated (eg $A_{wall}$=total dose/primary dose in CAVRZnrc, dose/KERMA in DOSRZnrc). In order to determine the uncertainties on these ratios, we use the following expression for the uncertainty on a ratio, C=X/Y:

$$\frac{s_{\overline{C}}}{\overline{C}} = \sqrt{\left(\frac{s_{\overline{X}}}{\overline{X}}\right)^2 + \left(\frac{s_{\overline{Y}}}{\overline{Y}}\right)^2 - \frac{2\mathrm{cov}(X,Y)}{(N-1)\left(\overline{X}\ \overline{Y}\right)}} \tag{5}$$

where $s_{\overline{X}}$ and $s_{\overline{Y}}$ are the uncertainties on $\overline{X}$ and $\overline{Y}$ as calculated using the history by history method outlined above, and cov(X,Y) is the covariance of X and Y, given by:

$$\mathrm{cov}(X,Y) = \frac{\sum_{i=1}^{N} X_i Y_i}{N} - \frac{\sum_{i=1}^{N} X_i \sum_{i=1}^{N} Y_i}{N^2} \tag{6}$$

Keeping track of $\sum_{i=1}^{N} X_i Y_i$ in the on the fly requires an additional `REAL*8` array for each ratio scored.

Both the batch method and the history by history method underestimate uncertainty if a phase space source file is restarted (which happens automatically if all particles in the source have been used). In the case of the history by history method, this is because particles that are re-used because of a restart are not associated with the same primary history as on the first pass through the source file, and thus correlations between these re-used particles are ignored. To overcome this problem, we recommend re-using each particle enough times before moving on to the next particle in the phase space source to avoid restarting the source. This re-use of particles "on the spot" is called particle recycling. To facilitate particle recycling we introduced the recycling number, `NRCYCL`, input with sources 21 and 22 (See Table 1). Each particle in the source will be used a total of `NRCYCL`+1 times before moving on to the next one. If the user sets `NRCYCL`<=0, then `NRCYCL` will automatically be calculated to sample the entire phase space source while avoiding a restart. The particle recycling scheme is identical to that currently in use in BEAMnrc and DOSXYZnrc.

For more information about history by history statistics and particle recycling, see Reference [11].

## 2.12 Internally used scoring arrays

The names of some of the variables used in the RZ codes to score quantities of interest are shown in Table 2.

Table 2: Variables used in AUSGAB to score quantities of interest. Z and R refer to the depth and radial zones. IQ refers to the charge of the particle involved and IT is defined in the last column. Note that scoring variables in CAVRZnrc do not have an IT mode. All variables shown are `REAL*8`

| User Code | Scoring Variable & description | Scoring Mode [IT] |
|---|---|---|
| DOSRZnrc | `SCDOSE(Z,R,IT)`:<br>stores energy deposited<br>in voxel (R,Z) summed over<br>all primary histories–after<br>analysis, stores dose in voxel | 1: Total dose<br>2: Stoppers and discards dose<br>3: Total dose from front wall<br>4: Total dose from outside wall<br>5: Total dose from back wall<br>6: Total dose from inside wall<br>7: Total dose scored in region NSRCRG due to electrons created in region |
| | `SCDOSE2(Z,R,IT)`:<br>stores (energy deposited in<br>voxel (R,Z))$^2$ summed over | same as above |

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| User Code | Scoring Variable & description | Scoring Mode [IT] |
|---|---|---|
| | all primary histories–after analysis stores uncertainty on dose in voxel | |
| | `SCKERMA(Z,R,IT)`: stores energy of electrons created in voxel (R,Z) summed over all primary histories–after analysis, stores kerma in voxel | 1: Kerma from primary photons<br>2: Kerma from scattered photons |
| | `SCKERMA2(Z,R,IT)`: stores (energy of electrons created in voxel (R,Z))$^2$ summed over all primary histories–after analysis, stores uncertainty on kerma in voxel | same as above |
| | `SCDOSEtoKERMA2((Z,R,IT)`: for voxel (R,Z), stores (energy deposited)*(energy of electrons created) summed over all primary histories–after analysis, stores uncertainty on dose/kerma in voxel | same as above |
| | `SCPDST(E)` and `SCPDST2(E)`: store sum of initial weight and (initial weight)$^2$ of primary histories whose total deposited energy in the pulse height region(s) falls in bin E–after analysis `SCPDST` stores the pulse height distribution and `SCPDST2` stores the uncertainty in `SCPDST` | N/A |
| | `SCPCUM(E)` and `SCPCUM2(E)`: store sum of initial weight and (initial weight)$^2$ of primary histories whose total energy deposited in the pulse height region(s) is $\leq$E–after analysis `SCPCUM` stores the cumulative pulse height distribution and `SCPCUM2` stores the uncertainty on `SCPCUM` | N/A |

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| User Code | Scoring Variable & description | Scoring Mode [IT] |
|---|---|---|
| | `SCDFEP(IPK)` and `SCDFEP2(IPK)`: store sum of initial weight and (initial weight)$^2$ of primary histories whose total energy deposited in the pulse height region(s) falls in peak IPK–after analysis `SCDFEP` contains contains fraction of primary histories depositing energy in peak IPK and `SCDFEP2` stores uncertainty on `SCDFEP` | IPK=1: incident energy peak<br>IPK=2: single-escape peak<br>IPK=3: double-escape peak<br>IPK=4: 0.511 MeV peak |
| | `SCDFBK(IPK)` and `SCDFBK2(IPK)`: store sum of initial weight and (initial weight)$^2$ of primary histories whose total energy deposited in the pulse height region(s) is in the background of peak IPK–after analysis, `SCDFBK` contains the no. of primary histories in the background and `SCDFBK2` contains the uncertainty on `SCDFBK`. `SCDFBK(IPK)` is subtracted from `SCDFEP(IPK)` in obtaining the final value of `SCDFEP(IPK)` | IPK same as above |
| | `SCDFDIFF(IPK)` and `SCDFDIFF2(IPK)`: stores difference in sum of initial weight and (initial weight)$^2$ between primary histories depositing energy in peak IPK and the background of peak IPK–used during analysis to determine covariance between `SCDFEP(IPK)-SCDFBK(IPK)` (peak - background) and the total no. of primary histories depositing energy in the pulse heigh regions. This allows `SCDFEP` to be expressed as a fraction of this total and the uncertainty, `SCDFEP2`, to be estimated properly. | IPK same as above |
| CAVRZnrc | `cav_dose`: stores energy deposited in cavity summed over all primary | |

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| User Code | Scoring Variable & description | Scoring Mode [IT] |
|---|---|---|
| | histories–after analysis, stores total dose in cavity | |
| | `cav_dose0`: similar to above, but for energy deposited by primary photons only | |
| | `cav_dose1`: same as `cav_dose0` but corrected for attenuation | |
| | `cav_dose2`: same as `cav_dose` but for energy deposited by secondary photons only | |
| | `cav2_dose`: stores (energy deposited in cavity)$^2$ summed over all primary histories–after analysis, stores uncertainty in cavity dose | |
| | `cav2_dose0`: same as `cav2_dose` but for primary photons only | |
| | `cav2_dose1`: same as `cav2_dose0` but corrected for attenuation | |
| | `cav2_dose2`: same as `cav2_dose` but for secondary photons only | |
| | `cav_dosec`: stores (energy deposited in cavity)*(energy deposited by unattenuated primaries in cavity) summed over all primary histories–after analysis, stores uncertainty on $A_{wall}$ | |
| | `cav_dosec01`: stores (energy deposited by primaries)*(energy deposited by unattenuated primaries) summed over all primary histories–after analysis stores uncertainty on $A_{att}$ | |
| | `cav_dosec02`: stores (energy deposited by primaries)*(energy deposited by secondaries) summed over all primary histories–after analysis stores uncertainty on $A_{scat}$ | |
| FLURZnrc | `SCFLU(E,Z,R,IQ,IT)` and `SCFLU2(E,Z,R,IQ,IT)`: store fluence and (fluence)$^2$ in energy bin E due to particles of charge IQ in voxel (R,Z) summed over all primary histories–after analysis, `SCFLU` stores the fluence in energy bin E in voxel (R,Z) due to particles of charge IQ and `SCFLU2` the uncertainty on `SCFLU` | 1: all particles<br>2: primary or scattered particles only |
| | `SCTFLU(Z,R,IQ,IT)` and | same as above |

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| User Code | Scoring Variable & description | Scoring Mode [IT] |
|---|---|---|
| | `SCTFLU2(Z,R,IQ,IT)`:<br>store total fluence and<br>(total fluence)$^2$ of particles<br>of charge IQ in voxel (R,Z) summed<br>over all primary histories–after analysis<br>`SCTFLU` stores the fluence of<br>particles of charge IQ in voxel (R,Z)<br>and `SCTFLU2` stores the uncertainty on<br>`SCTFLU` | |
| | `SCEAVE(Z,R,IQ,IT)` and<br>`SCEAVE2(Z,R,IQ,IT)`:<br>store energy and (energy)$^2$<br>of particles of charge IQ crossing<br>voxel (R,Z) summed over all primary<br>histories–after analysis `SCEAVE`<br>stores the average energy of particles<br>of charge IQ crossing (R,Z) (computed by<br>dividing `SCEAVE(Z,R,IQ,IT)` by<br>`SCTFLU(Z,R,IQ,IT)`) and `SCEAVE2`<br>stores the uncertainty on `SCEAVE` | 1: all particles<br>2: primary or scattered particles |
| | `SCTLEP(Z,R,IT)` and<br>`SCTLEP2(Z,R,IT)`:<br>store total fluence and<br>(total fluence)$^2$ of charged<br>particles in voxel (R,Z) summed<br>over all primary histories–after<br>analysis `SCTLEP` stores the total<br>fluence of charged particles in (R,Z)<br>and `SCTLEP2` the uncertainty on<br>`SCTLEP` | same as above |
| | `SCELEP(Z,R,IT)` and<br>`SCELEP2(Z,R,IT)`:<br>store energy and (energy)$^2$<br>of charged particles crossing<br>voxel (R,Z) summed over all<br>primary histories–after analysis<br>`SCELEP` stores average energy of<br>charged particles crossing (R,Z)<br>(calculated by dividing `SCELEP(Z,R,IT)`<br>by `SCTLEP(Z,R,IT)`) and `SCELEP2` | same as above |

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| User Code | Scoring Variable & description | Scoring Mode [IT] |
|---|---|---|
| | stores the uncertainty on SCELEP | |
| | SCFLEP(E,Z,R,IT) and SCFLEP2(E,Z,R,IT): store fluence and (fluence)$^2$ of charged particles in energy bin E in voxel (R,Z) summed over all primary histories–after analysis SCFLEP stores fluence of charged particles in energy bin E in voxel (R,Z) and SCFLEP2 stores the uncertainty on SCFLEP | same as above |
| | SCEAVE_COV(Z,R,IQ,IT): stores (energy of particles of charge IQ crossing voxel (R,Z))*(total fluence of particles of charge IQ in voxel (R,Z)) summed over all primary histories. Used to calculate covariance term for uncertainty in final value of SCEAVE(Z,R,IQ,IT) (see above) | same as above |
| | SCELEP_COV(Z,R,IT): stores (energy of charged particles crossing (R,Z))*(total fluence of charged particles crossing (R,Z)) summed over all primary histories. Used to calculate covariance term for uncertainty in final value of SCELEP2(Z,R,IT) (see above) | same as above |
| SPRRZnrc | SCEDPN(Z,R,IT) and SCEDPN2(Z,R,IT): store energy deposited and (energy deposited)$^2$ in voxel (R,Z) summed over all primary history–after analysis SCEDPN2(Z,R,1) stores stopping power ratio (local medium/MED2) including stoppers. SCEDPN2(Z,R,3) stores the stopping power ratio excluding stoppers. SCEDPN2(Z,R,1) | 1: in local material excluding brem created below PCUT, atomic relaxations and electrons created below ECUT, but includes electrons slowing down across ECUT (stoppers)<br>2: in second material (MED2) with transport in local material<br>3: same as 1 but without stoppers<br>4: same as 2 but without stoppers |

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| User Code | Scoring Variable & description | Scoring Mode [IT] |
|---|---|---|
| | stores uncertainty in `SCEDPN(Z,R,1)` and `SCEDPN2(Z,R,3)` stores uncertainty in `SCEDPN(Z,R,3)` | |
| | `SCDOSE(Z,R,IT)` and `SCDOSE2(Z,R,IT)`: store energy deposited and (energy deposited)$^2$ in voxel (R,Z) summed over all primary histories–after analysis, `SCDOSE(Z,R,IT)` contain dose in voxel (R,Z). For IT=1,2 these are expressed as fractions of the total dose (IT=3). `SCDOSE2(Z,R,IT)` contains uncertainty in `SCDOSE(Z,R,IT)`. | 1: stoppers only<br>2: brems created below PCUT, atomic relaxations and electrons created below ECUT<br>3: total |
| | `SCSPR_COV(Z,R,IT)`: stores (energy deposited in local medium)*(energy deposited in MED2) in voxel (R,Z) summed across all primary histories. Used to calculate covariance for uncertainties in final value of `SCEDPN2(Z,R,1)` and `SCEDPN2(Z,R,3)` | 1: including stoppers<br>2: excluding stoppers |
| | `SCDOSE_COV(Z,R,IT)`: stores (total energy deposited)* (energy deposited indicated by IT) summed over all primary histories. Used to calculate covariance for uncertainties in final values of `SCDOSE(Z,R,IT)` for IT=1,2 (recall that these are expressed as fractions of total dose | 1: stoppers only<br>2: brems created below PCUT, atomic relaxations and electrons created below ECUT |

After the completion of a batch, the `.egsdat` file will be updated and will contain the complete scoring arrays, random generator state, etc calculated so far, and consequently, a run can be restarted from that point on. So although the batch results are no-longer used for statistical analysis, the calculations are still done in 10 batches to facilitate storage of partial results.

## 2.13 Compiling and running the codes

The EGSnrcMP RZ codes can all be compiled and run using the GUI which is invoked by typing `egsinprz` or by clicking on the GUI icon (see the GUI Manual [5] for more information). They can also be compiled at the same time as you install the EGSnrcMP system. You can, however, compile and run them using the standard commands for compiling and running user codes described in detail in the EGSnrcMP manual [1]. These commands will be summarized briefly here.

### 2.13.1 Compilation

The RZ codes are compiled using the `make` utility. Before compiling a code, copy the files:

```
Makefile
user_code.mortran
user_code.make
user_code.io
```

from `$HEN_HOUSE/user_code` into your `$EGS_HOME/user_code` directory (creating this latter directory if it does not exist). Note that the file `user_code.io` is not used during compilation, but will be used when you run the code.

Once you have successfully copied these files, go into directory `$EGS_HOME/user_code` and type:

```
make [options]
```

The options for `make` are:

```
make              Compile with default optimization
make opt          turned on.  Default optimization is level 2 (-O2).

make noopt        Compile with no optimization

make debug        Compile executable for debugging.

make fortran      Do mortran compilation only, leaving behind the Fortran
                  file user_code.F.

make clean        Remove the Fortran file, mortjob.mortran file,
                  user_code.mortlst file and the executable.
```

To preserve compatibility with old usage, the `mf` command is also available for compiling user codes on a Linux/Unix system (you must have sourced `$HEN_HOUSE/scripts/egsnrc_cshrc_additions` or `$HEN_HOUSE/scripts/egsnrc_bashrc_additions` from your `.cshrc` or `.bashrc` file). `mf` is aliased to the script `$HEN_HOUSE/scripts/compile_user_code`.

To use `mf`, go into `$EGS_HOME/user_code` and type:

```
m[f] user_code [a] [opt|noopt|debug]
```

The options for `mf` are: `mf` => Mortran and Fortran compile and then link
`m` => Mortran compile and create the Fortran file
`opt` => use optimization (default level 2)
`noopt` => use no optimization
`debug` => create executable ready for a debug run
The parameter "`a`" is not used and is only present for compatibility with the previous version of `mf`.

Once you have successfully compiled the RZ code, the executable, `user_code*`, will be left in your `$EGS_HOME/bin/config` directory (where `config` is the name of the configuration that you are using).

### 2.13.2 Execution

To run any of the RZ codes interactively from the command line type

```
user_code -i inputfile -p pegsdata
```

where the input file is `$EGS_HOME/user_code/inputfile.egsinp` and the file `pegsdata.pegs4dat` contains the PEGS4 data set (it can be on `$EGS_HOME/pegs4/data` or if not found there, on `$HEN_HOUSE/pegs4/data`).

If you are using a Unix/Linux system, then you can also start an interactive run using the `ex` (aliased to `$HEN_HOUSE/scripts/run_user_code`) command:

```
ex user_code inputfile pegsdata
```

`ex` is provided to preserve compatibility with old usage.

If you are running on a Linux/Unix system, then you can run the RZ codes in batch mode. Batch mode is required for parallel runs (see section 2.14 below for more information on this). Batch submission uses the `exb` command, which is aliased to the script `$HEN_HOUSE/scripts/run_user_code_batch`. The syntax of the `exb` command is:

```
exb user_code inputfile pegsdata [short|medium|long] [batch=batch_sys]
```

`[short|medium|long]` is an optional input indicating which queue to use (default is `long` if not specified). You can change the names of the queues that `short`, `medium` and `long` are mapped onto in the file `$HEN_HOUSE/scripts/batch_options.batch_sys`. The `batch_sys` input defines the network queuing system to use. Currently, `batch_sys` can be set to `at` (the standard Unix batch command), `pbs` (to use PBS), `keg` (to use Sun's SGE) or `nqs` (for NQS). The default is `at` unless otherwise specified by setting the environment variable `$EGS_BATCH_SYSTEM`.

Once an interactive or batch run is started, a temporary working directory is created as a subdirectory of `$EGS_HOME/user_code`. This temporary working directory has the name `egsrun_pid_inputfile_hostname`, where where `pid` is the process ID number and `hostname` is the name of the computer you are submitting the job from. All output files are written to this temporary directory. At the end of the run, the files are moved into `$EGS_HOME/user_code`

and the temporary working directory is deleted. For more information on temporary working directories, see the EGSnrcMP Users Manual[1].

## 2.14 Parallel processing

Previously, parallel processing with the RZ codes used the Unix `pprocess` script, which created separate input files for each job, with the same number of histories (total histories/no. of jobs) in each job. These input files were then submitted to the batch queueing system. This approach has a major limitation in that the calculation is only as efficient as the fastest CPU used.

The `pprocess` script is still available, however we recommend using the new parallel processing functionality built in to EGSnrcMP. This is documented in more detail in the EGSnrcMP manual [1], however a brief description will be given here. In order to make use of this functionality, you must be running on a Unix/Linux machine with a batch queuing system (eg PBS or NQS) and have installed EGSnrcMP with a working C/C++ compiler.

### 2.14.1 Submitting parallel jobs

To submit a parallel job, use the `exb` command with the following syntax:

```
exb user_code inputfile pegsdata [short|medium|long] batch=batch_sys [p=N] \
    [start=i_start-1] [stop=i_stop]
```

`p` specifies the number of parallel jobs (defaults to `i_stop-i_start+1`), `start` is an input to set the index number of the first parallel job (defaults to 1), and `stop` sets the index of the last parallel job (defaults to `i_start+N-1`). Note that if `stop` is not set, then `p` must be set and `stop` takes on its default value. If `p` only is set (a common practice), then the jobs are numbered 1,...,`N`. It is possible to set all three inputs with `i_stop-i_start+1<N`, in which case the code will behave as if a subset of the full `N` parallel jobs is being run. This may be useful if there is a delay between submitted portions of the full complement of parallel jobs. Other input parameters are the same as described in section 2.13.2. Recall that the default value of `batch_sys` is `at` (the standard Unix batch command), however parallel jobs will not run with `at`. Thus, you must either explicitly input `batch_sys` above or else set the environment variable `$EGS_BATCH_SYSTEM`, to something other than `at`.

Parallel jobs are controlled by a job control file, `$EGS_HOME/user_code/inputfile.lock` (automatically created by the first job submitted). This file is read from and updated by all parallel jobs and contains the total number of histories remaining to be run and the number of jobs running, among other information. Jobs run until there are no histories remaining in the job control file. Rather than each job running a fixed (`NUMBER OF HISTORIES`)/`N` histories (as in the old `pprocess` scheme), a job is only allowed to run a fraction, or "chunk" of this number at a time. Thus each run consists of (`NUMBER OF HISTORIES`)/(`N`*`$N_CHUNK`) histories, where `$N_CHUNK` is defined in `$HEN_HOUSE/src/egsnrc.macros` and is set by default to 10. Breaking the simulation into smaller chunks allows jobs using faster CPU's to run more histories than those running on slower CPU's, increasing the efficiency of this new parallel processing scheme.

Each parallel job outputs the same files that the simulation would have if not run in parallel, only instead of being named `inputfile.ext` (where `ext` is `egslst`, `egsdat`, `plotdat`, etc), they are named `inputfile_w[i_parallel].ext`, where `i_parallel` is the index number of the job (`i_start`,`i_start+1`,...,`i_start+N-1`).

If a parallel job finds there are no histories left to run in `inputfile.lock`, then it analyzes the results for its own runs and outputs the results to its `inputfile_w[i_parallel].egslst`, `inputfile_w[i_parallel].plotdat`, etc, files.

### 2.14.2 Random number seeds for parallel jobs

Each of the parallel jobs must begin with a different random number seed. This is accomplished by incrementing the second random number seed, `JXXIN` (see section 2.10.2 above), for each parallel job submitted using:

$$\texttt{JXXIN} = \texttt{JXXIN}_{input} - 1 + \text{i\_parallel} \tag{7}$$

where $\texttt{JXXIN}_{input}$ is the value of `JXXIN` in `inputfile.egsinp` and `i_parallel` is the parallel job number (`i_start`,`i_start+1`,...,`i_start+N-1`).

### 2.14.3 Phase space sources and parallel jobs

If you are using a phase space file as a source (source 21 or 22 – see section 2.7), then this source is partitioned so that it is sampled evenly over all jobs. Each chunk of the run uses a different partition of the phase space file, where the number of particles in each partition `P_PER_PHSP_CHUNK`, is given by:

$$\texttt{P\_PER\_PHSP\_CHUNK} = \frac{\texttt{NCASE\_PHSP}}{(\texttt{N*\$N\_CHUNKS})} \tag{8}$$

where `NCASE_PHSP` is the total number of particles in the phase space source.

### 2.14.4 Combining results of parallel runs

The last parallel job to end calls a subroutine in the user code (`combine_results`) which reads and sums the data stored in the `inputfile_w[i_parallel].egsdat` files from the parallel jobs. These combined results are then analyzed and output to the `inputfile.egslst` file along with any other output files you may have selected (e.g. `inputfile.plotdat`). Note that this means that to combine parallel runs, you must always have `STORE DATA ARRAYS= YES` (see section 2.9.4) so that the `.egsdat` files are output.

The `inputfile_w[i_parallel].egsdat` can also be manually combined by rerunning your code with the input parameter `IRESTART= PARALLEL`. This may be useful if you want to combine results from several different groups of parallel runs.

This system of combining results works very well unless you have huge `.egsdat` files (can happen with FLURZnrc), in which case you can quickly run out of disk space and or bring your network to its knees.

### 2.14.5 Restarting parallel runs

Parallel jobs can be restarted the same way as a single run, by rerunning with `IRESTART=restart` (see section 2.9.3) in `inputfile.egsinp`. Note that all of the `.egsdat` files from the previous parallel jobs must be available and you must submit the same number of parallel jobs beginning with the same value of `i_start` (see section 2.14.1 above). If you are using a phase space source, however, restarting presents a problem in that a particular partition of the source may get used by a different job the second time around. At the end of the run, results from the second use of this partition will be recombined with those from its first use with no attention paid to the correlation between the two results. This will result in the uncertainties being underestimated. We recommend that you do not restart a parallel run if you are using a phase space source.

If you are restarting a parallel run that uses a full BEAMnrc simulation source (source 23–See Section 2.7). Then you must go into the input file for the simulation source and set the input variable `IRESTART` to 1. Otherwise, the simulation source in the restarted run will use identical random numbers as in the original run.

## 2.15 Pegsless Mode

The user has the option of running EGSnrc user codes in pegsless mode, thus eliminating the requirement for a-priori calculation of cross-section data and generation of a `.pegs4dat` file. Photon interaction cross-sections have been calculated on-the-fly since 2006. Thus, the migration to a fully pegsless implementation of EGSnrc required that the calculation of electron cross-sections be similarly done on a simulation-by-simulation basis.

### 2.15.1 Pegsless Inputs

To run in pegsless mode, the user must include parameters for calculating cross-sections, including specifications for all media used in the simulation, in their `.egsinp` file between the delimiters, `:start media definition:` and `:stop media definition:`. This is best illustrated with an example input:

```
:start media definition:

AE=0.521
UE=50.511
AP=0.01
UP=50.

material data file=/home/username/HEN_HOUSE/pegs4/data/material.dat

:start H2O521ICRU:
  elements = H, O
  number of atoms = 2,1
  rho = 1.0
```

```
  bremsstrahlung correction = KM
:stop H2O521ICRU:

:start AIR521ICRU:
  elements = C,N,O,AR
  mass fractions = 1.24000E-04, 7.55200E-01, 2.31800E-01, 1.28300E-02
  rho = 1.2048E-03
  bremsstrahlung correction = NRC
  gas pressure = 1.0
:stop AIR521ICRU:

:start PMMA521ICRU:
  bremsstrahlung correction = NRC
  density correction file = /home/uname/EGSnrc/HEN_HOUSE/pegs4/density_corrections/
compounds/polymethylmethacrylate__lucite___perspex___plexiglas_.density
:stop PMMA521ICRU:

:stop media definition:
```

where:

`AE,UE,AP,UP` are the kinetic energy limits for calculating photon (`AP,UP`) and electron (`AE,UE`) cross sections in MeV. These energy limits are also mentioned in the context of the EGSnrc system in Section **??**. If `AE` is not specified it defaults to the highest value of `ECUT` (electron transport cutoff energy–see Section **??**) specified in the simulation. If `AP` is unspecified, then it defaults to the highest value of `PCUT` (photon transport cutoff energy–see Section **??**) specified. `UE` and `UP` default to 50.511 MeV and 50.0 MeV, respectively.

`material data file` is the name (including full directory path) of a file containing specifications for the media used in the simulation. Provided with the EGSnrc distribution is the material data file `$HEN_HOUSE/pegs4/data/material.dat` which contains specifications necessary to reproduce all of the cross-section data in `521icru.pegs4dat` and `700icru.pegs4dat` (provided that the appropriate values of `AE, UE, AP and UP` are specified–see above). Note that the format for media specifications in the material data file is similar to that used for specifying media directly in the `.egsinp` file, described immediately below. In the case of the material data file, however, there is some redundancy in the specification to allow the user to see the composition and density of the media.

the `:start MEDNAME:` and `:stop MEDNAME:` delimiters are used to specify medium, `MEDNAME`, directly in the `.egsinp` file. This method of specifying a medium is used if `MEDNAME` is not included in the material data file or if you wish to override some or all of the specifications for `MEDNAME` in the material data file. If no material data file is input, then all media in the simulation must be specified in this way. The inputs between these delimiters are described below. Variables in square brackets are the analogous PEGS4 variables described in the PEGS4 Manual (Section **??**) above.

`elements` specifies the elements comprising the medium. Elements are specified using chemical symbols separated by commas. Case is unimportant.

`number of atoms` [`PZ`] or `mass fractions` [`RHOZ`]. For each of the `elements`, specify either the number of atoms in a molecule of the medium (*i.e.* stoichiometric coefficients), if the medium is a compound, or the mass fractions of the elements in the medium, if the medium is a mixture. Values are separated by commas and are input in the same order as their corresponding elements. In the example above, the composition of `H2O521ICRU` is defined using the number of atoms of each element, while that of `AIR521ICRU` is defined using the mass fraction of each element. Note that this input is omitted if the medium is an element.

`rho` specifies the bulk density of the medium in g/cm$^3$.

`bremsstrahlung correction` [`IAPRIM`] specifies the correction to apply to calculated bremsstrahlung cross-sections. Options are:

- `KM` [IAPRIM=0] (the default): Apply Koch and Motz[13] empirical corrections.
- `NRC` [IAPRIM=1]: Apply NRC corrections based on NIST/ICRU[14]. These corrections are read from the file `$HEN_HOUSE/pegs4/aprime.data`.
- `None` [IAPRIM=2]: No corrections applied.

`density correction file` [`EPSTFL`] is the name of a file containing density effects which, when applied to calculated collision stopping powers, results in agreement with collision stopping powers published in ICRU37[15]. In general, density correction files are specified including their full directory path and `.density` file extension. However, the file can be specified by its prefix only if it exists in, in order of search priority:

1. `$EGS_HOME/pegs4/density_corrections`
2. `$EGS_HOME/pegs4/density_corrections/elements`
3. `$EGS_HOME/pegs4/density_corrections/compounds`
4. `$EGS_HOME/pegs4/density`
5. `$HEN_HOUSE/pegs4/density_corrections/elements`
6. `$HEN_HOUSE/pegs4/density_corrections/compounds`

Note that the density correction files for many elements, compounds and mixtures are supplied with the distribution. Density correction files have a header portion from which the composition and bulk density of the medium are read. These values override any user inputs for `elements=`, `number of atoms=` or `mass fractions=`, and `rho=`. Thus, as in the case of `PMMA521ICRU` in the example above, it is possible to specify the composition of a medium simply by specifying a density correction file.

`gas pressure` [`GASP`] is the pressure of the medium in atm if the medium is a gas. This input is only relevant (and necessary for a gas) if a density correction file is not used, in which case `gas pressure` is used to modify the calculated density effect parameters. `gas pressure` defaults to 0 (*i.e.* the medium is not a gas).

Inputs specifying media are case insensitive with the exception of the medium name (*e.g.* `H2O521ICRU` is different than `h2o521ICRU`).

### 2.15.2 egs_inprz GUI

The user has access to the pegsless inputs described above through the GUI for the RZ user codes, `egs_inprz`. By selecting the "Go PEGSless" radiobutton on the first page of the GUI ("General" inputs tab), the user enables a "Media Definition" tab. Opening this tab, the user can add/modify the cross section energy limits (`AE, UE, AP, UP`), the name of the material data file and the specifications for media defined directly in the `.egsinp` file. New media can be specified in the `.egsinp` file by selecting "define new medium" in the "medium name" list box and then entering the name of the new medium. Note that in order to add the new medium to the list, you must hit <`return`> after typing its name. Media can be deleted from the list of media in the `.egsinp` file by deleting their name and then selecting away from them in the "medium name" list box. The name of the medium and its associated specifications (composition, bulk density, etc) will be deleted.

### 2.15.3 Running in Pegsless Mode

EGSnrc user codes can be run interactively in pegless mode using the command line input:

```
user_code -i inputfile
```

where `inputfile` is the name of the inputfile (with no `.egsinp` extension).

Pegsless batch runs use the command line syntax:

```
exb user_code inputfile pegsless [short|medium|long] [batch=batch_system] [p=N]
```

This is identical to the syntax of a run with pegs data (see Section 2.14.1 above) but with the word `pegsless` in place of the name of the pegs data file.

When running in pegsless mode, EGSnrc outputs a file, `inputfile.mederr`, which, for each medium used in the simulation, indicates where each specifying parameter has been read (*i.e.* from a material data file or directly from the `.egsinp` file). The file also includes warnings when `AE`, `UE`, `AP` or `UP` have not been specified and have been set to their default values and when a material data file has not been specified. For parallel runs in pegsless mode (parameter `p` $> 1$ in the batch command syntax above), the `.mederr` file is only output by the first job.

The actual values of the media specifications (including defaults) used to calculate cross-sections are output in the listing file, `inputfile.egslst`, and to the screen for interactive runs or in the log file, `inputfile.egslog`, for batch runs.

## 2.16 Standard I/O Units

The following files are associated with a normal type of run with an NRC user code, although the `user_code.io` file can add whatever files the user may want and the files below are not mandatory. See section 2.17 below for more details. For this example, the input file name is `input.egsinp`.

**input.egsinp:** defined by the user.

**input.egslst:** the output listing file from the run. Erased at start of next run if not renamed.

**input.egslog:** The log file which echos the inputs and prompts when running in batch. Note, this has most of the **error** messages too, so get in the habit of reading this file.

**input.egsdat:** A file containing all the information needed to allow a calculation to be restarted again.

**input.egsrns:** Some codes allow a record of random number seeds at the start of every history or the last history to be kept. These are kept in this file if requested. It can be useful for debugging.

**input.plotdat, input.spectra, input.plotphd:** Plotting files for various routines readable by `xmgrace`. `input.plotdat` generally holds dose, fluence or stopping-power ratio plots. `input.spectra` holds fluence spectra plots (FLURZnrc only). `input.plotphd` holds pulse height distribution plots (DOSRZnrc only).

**input.egseff:** Tabulated form of pulse height distribution (DOSRZnrc only).

**input.egsgeom:** file with output description of geometry for `EGS_windows`.

**input.egsgph:** file with output phase space of each history for `EGS_windows`.

**input.errors:** file contains warning and error messages from the GET_INPUT routine. This file is also in the `.egslog` file at the end.

**input.eo:** file contains output from the batch queuing system (e.g. PBS or NQS). This file is only output if the job has been run in batch mode.

If you want to modify the user codes and need more files, these can be defined via the `user_code.io` file (see section 2.17 below).

## 2.17 The `.io` file

Output files are associated with standard Fortran units (i.e. `fort.*`) using the `user_code.io` file located in `$EGS_HOME/user_code`. An typical `.io` file (`dosrznrc.io`) contains:

```
1  .egslst
15 .errors
```

The left column is the Fortran unit number and the right column is the file extension (added to `inputfile`). For example, in this case `fort.1` is the file `inputfile.egslst`.

Files associated with Fortran units in `user_code.io` are opened in subroutine `egs_init`, called at the beginning of the RZ code, and are closed in subroutine `egs_finish`, called at the end of the code. Both of these subroutines are in the file `$HEN_HOUSE/src/egs_utilities.mortran`. Files in `user_code.io` are opened unconditionally. Output files that are only created if certain input parameters are set must be opened and closed explicitly in the user code.

## 2.18 Makefile and user_code.make

Before compiling an RZ code using the make command, you must have copied both Makefile and user_code.make from $HEN_HOUSE/user_code into your $EGS_HOME/user_code directory. Makefile can be seen as the "master" file directing the compilation. In the case of the RZ codes, Makefile directs the compilation to include the files $HEN_HOUSE/specs/config.conf (defines the compiler name and default compiler options for the system, config, that you are running on), user_code.make (more about this below) and $HEN_HOUSE/makefiles/standard_makefile (defines compilation rules, dependencies and the make options discussed in section 2.13.1 above). Makefile also defines the variable USER_CODE (i.e. sets it to dosrznrc, flurznrc, cavrznrc or sprrznrc) which is used in standard_makefile.

The user_code.make file defines several variables:

EGS_EXTRA_OBJECTS **and** EGS_EXTRA_LIBS C and Fortran object and library files to be linked at compile time. Files are referred to by variable names which are defined in $HEN_HOUSE/specs/config.conf and depend on what type of machine you are running on and whether or not you have a working C/C++ compiler. In particular, the C files are necessary to make use of the built-in parallel processing functionality (see section 2.14) and to use a BEAM simulation as a source (source 23, see section 2.7).

RANDOM Defines the random number generator to be used. This can be set to either $(EGS_SOURCEDIR)ranmar (default) or $(EGS_SOURCEDIR)ranlux to use the RANMAR or RANLUX random number generator respectively (see section 2.10.2 for more on the RNGs).

SOURCES Defines the MORTRAN source (macro and code) files that are concatenated together (and the order in which they are concatenated) to create the mortjob.mortran file that is ultimately compiled. You can make changes to SOURCES to include additional files or change the directory where a source file is pulled from. Note that the order of the macro files is important since a macro must be defined before it is used in a code and, in the case of multiple definitions of a macro, the last definition is the one used.

For more information on Makefile and user_code.make, see the EGSnrcMP Manual [1].

## 2.19 Miscellaneous general information/inputs

### 2.19.1 Normalization of output

One must be careful of how the results are normalized in the codes. It differs in the various codes and also differs depending on the source option being used.

Table 3 below summarizes how output quantities are normalized for each source type.

Table 3: Normalization of output values for all sources.
See Table 1 for a description of the sources.

| Source No. | Description | Normalization |
|---|---|---|
| 0 | Parallel beam incident on front | planar fluence on front face (ie not corrected for incident angle) |
| 1 | Point source on axis from front | fluence on front face at central axis |
| 2 | Broad parallel beam from front | planar fluence in beam |
| 3 | Isotropically-radiating internal source | initial particles |
| 4 | Central axis depth-dose vs beam radius | incident particles |
| 10 | Parallel beam incident from side | planar fluence of beam |
| 11 | Point source incident from side | fluence at central (Z) axis |
| 12 | Point source off axis | fluence at centre of geometry |
| 13 | Parallel beam from any angle | fluence on cylinder |
| 14 | Point source on z axis excluding events inside RMINBM | fluence on front face |
| 15 | Point source from any angle | fluence at centre of geometry |
| 16 | Circular or rectangular isotropically-radiating source from any angle | fluence at centre of geometry |
| 20 | Radial distribution input | fluence on front face (assumes uniform distribution over all radii) |
| 21 | Phase space source from front | incident particles from original, non-phase-space source |
| 22 | Phase space source from any angle | incident particles from original, non-phase-space source |
| 23 | Full BEAM simulation from any angle | incident particles from primary BEAM source |

The most common output is a quantity per unit incident fluence (e.g. dose per unit incident fluence in Gy-cm$^2$). The issue is about where the incident fluence is defined. This is not always the same and one must be careful.

For most parallel beams the fluence in the beam is independent of position and does not take into account the angle of incidence on the geometry (except source 13).

Point source routines are more complex. For a point source on the Z-axis, the incident fluence is defined on the central axis at the outer planar face of the cylinder with the lowest Z-value. If the point source is very close to the cylinder, this number is not immediately obvious.

Once a point source moves off the Z-axis the fluence is defined "at the midpoint of the cylinder". Thus two runs using source 1 and source 12 with the points very close to each other, could still be normalized quite differently if the cylinder were very long.

For the isotropically radiating internal source and the phase space sources the final normalization is given in terms of the number of initial particles and is no longer directly related to fluence.

# 3 DOSRZnrc

## 3.1 Introduction

This code simulates the passage of an electron or photon beam in a finite, right cylindrical geometry. It also scores pulse height distributions in an arbitrary volume made up of any number of regions. There is a write to unit 22 (`.plotphd`) of the calculated spectra/response functions although there are additional restrictions if the pulse height distribution is being scored. The energy deposited within various user defined regions is scored and analyzed statistically following the simulation. This code is the work-horse dose scoring code developed and used extensively at NRC. All other RZ codes are very similar in many ways.

This code and its ancestors, (DOSRZ, JACKET, INHOM), have been used in many publications and verified in many situations[16, 17, 18, 19, 10, 8, 20]. One must be aware that there are small but real differences between EGSnrc results and EGS4 results with this code (see ref [21]).

## 3.2 User Controls

The user has controls over the geometry, materials and simulation by:

1. defining the geometry of the target via the input of a number of planar and cylindrical coordinates which divide the cylinder into a number of regions, each region composed of a user specified material.
2. specifying in which of these regions the dose is to be scored.
3. selecting the form and degree of detail of the output.
4. selecting either the energy if a monoenergetic beam is to be used, or specifying ithe filename of a file containing an energy spectrum consisting of energy bins and corresponding probabibities
5. selecting the source of radiation from amongst parallel and point sources originating from the side or front, isotropically radiating sources embedded in regions in the cylinder and phase space files from BEAM.
6. selecting the number of histories, time limit and statistical limit. All histories will be run unless time runs out or the variance calculated in the peak region drops below the statistical limit.
7. selecting transport controls such as the fractional energy loss per charged particle step, the maximum step size, particle energy cutoffs, range rejection parameters.

## 3.3 Output

The first section of the output (in the `.egslst` file) echos the user input. The second section is messages and information printed during the simulation as a means of monitoring the simulation. The third section details the doses scored with accompanying statistical uncertainties. The first and third sections may include grid format summaries if requested by the user. Plot files are also output.

## 3.4 Input/output control

I/O control input in DOSRZnrc is delimited between `:start I/O control:` and `:stop I/O control:`. In addition to the I/O control inputs common to all codes (see section 2.9(page 35)), DOSRZnrc has the following I/O inputs:

```
OUTPUT OPTIONS
      = short                       (0)  short output -just dose grid(DG)
      = dose summary                (1)  output dose summary only (DS)
      = material summary            (2)  output material grid(MG) & DG
      = material and dose summary   (3)  output MG + DS
      = long                        (4)  output MG + DS + DG
                          Note-any time there is a dose summary, there
                          is also an .egsdose file, unit 10
                          [IOOPTN]

ELECTRON TRANSPORT
      = normal           (0) normal electron transport
      = no interactions  (1) no discrete interactions (used for CDSA
                             calculations but note that special data
                             sets are also needed to do a proper CSDA
                             calculation. All turning off interactions
                             does is just that. See use of IUNRST=2,3,4
                             PEGS4 data sets for real CSDA.)
                          [ ICSDA]
```

For complex geometries you may want just to output the doses in a few regions. These are defined using dose bounds. Note that proper transport is done everywhere and this is NOT related to range rejection, it is just an output option. Values which are too large are reduced to the maximum region used in the calculation.

```
  DOSE ZBOUND MIN    (I) Minimum plane # defining dose region (default=1)
                         [NZDMIN]
  DOSE ZBOUND MAX    (I) Maximum plane # defining dose region
                         [NZDMAX]
  DOSE RBOUND MIN    (I) Minimum cylinder # defining dose region (default=0)
                         [NRDMIN]
  DOSE RBOUND MAX    (I) Maximum cylinder # defining dose region
                         [NRDMAX]
```

### 3.4.1 How to do a CSDA calculation

To do a CSDA calculation one needs to prepare data sets using `IUNRST = 2` in the PEGS4 input files. This provides unrestricted stoipping powers and effectively infinite mean free paths to discrete interactions. This CSDA calculation deposits all bremsstrahlung on the spot. Since this essentially leaves no energy loss straggling in the EGSnrc calculation, the calculation is not very realistic. Using other values of `IUNRST` in PEGS4 one can get other variations of CSDA calculations (see section 6.1.1 of the EGSnrc manual).

A meaningful CSDA calculation with EGSnrc awaits implementation of energy loss straggling for the sub-threshold events.

## 3.5 Monte Carlo control

Monte Carlo control input is delimited between `:start Monte Carlo inputs:` and `:stop Monte Carlo inputs:`. In addition to the Monte Carlo control inputs common to all codes (see section 2.10, DOSRZnrc has the following Monte Carlo input parameters (which are discussed more fully below):

```
IFULL
       = dose and stoppers (0) just calculate total dose and that due
                               to stoppers and discards.
       = entrance regions  (1) as well analyze the total dose per
                               entrance region.
       = pulse height      (2) score a pulse height distribution in
         distribution          the volume specified after the
                               material inputs.
       = scatter fraction  (3) score the scatter fraction instead of
                               stoppers.  Only for incident photons.
                               Dose after Compton and for fluorescent
                               photons if followed.

STATISTICAL ACCURACY SOUGHT(R) % statistical accuracy of the total
                               dose in the peak region that is sought
                               The program executes until this
                               accuracy is obtained or the CPU time
                               runs out. If 0, no effect.

SCORE KERMA
      = no         (0) do not score kerma
      = yes        (1) score kerma wherever dose scored and estimate
                       ratio of dose/kerma using correlated uncertainty
                       estimate. This only makes sense for photon beams.
                       [IKERMA]
```

### 3.5.1 Scoring dose components(IFULL)

IFULL= dose and stoppers
DOSRZnrc will output the total dose and the total dose minus dose due to stoppers and discards within each region. This is the default output option. Stoppers and discards are particles whose histories have been terminated in that region for some reason, *eg.* because E(NP) $<$ ECUT,PCUT or E(NP) $<$ AE,AP. This can be a useful diagnostic. If the stoppers dose is a large fraction of the total, this means that electrons are not being transported much in that region.

IFULL= entrance regions
DOSRZnrc will output the total dose in each region along with the fractions of the total dose due to electrons entering from the front, back, inside and outside walls of the region. Any fraction of the dose not accounted for by these four entrance walls is assumed to come from electrons that originated in the region.

IFULL = pulse height distribution
The response function for a given set of regions will be scored (see reference[16] for a discussion of response functions). Specification of the input for the scoring of such distribution is delimited between :start pulse height distribution input: and
:stop pulse height distribution input:. It contains the following parameters:

```
REGION OF SENSITIVE VOLUME     Region numbers(IRL) of sensitive volume

SLOTE  (R)   for the pulse height distribution, defines the
             output energy bins. For SLOTE > 0.0, use equal size
             bins of this width in MeV (this will get increased
             by  factors of two until the whole initial spectrum is
             covered.
             SLOTE < 0.0, flags additional input: 'TOPS OF ENERGY BINS'

DELTAE (R)   code analyses peak efficiencies using a bin width
             of 2*deltae about each peak and two background regions
             of width deltae above and below the peak. default
             value is 0.005 MeV (no meaning for electrons, positrons)

IF SLOTE < 0.0 Input tops of individual energy bins for pulse height
               distribution using:
   TOPS OF ENERGY BINS        lowest energy first, tops of bins.
              [BINTOP]
```

Using SLOTE, described above, incident particles are binned according to the total energy that they have deposited in the sensitive volume. The pulse height distribution is output to the .egslst file. Here, it is normalized so that counts/bin add up to 1. The distribution is also output, in tabular form, to the .egseff file, with the number of counts in each bin having been divided by the bin width (in MeV) to give counts/MeV. Finally, the pulse height distribution is also output (in counts/MeV) to the .plotphd form for plotting using xmgrace or a similar plotting package. In both .egslst and .egseff files, the pulse height

distribution is accompanied by calculated peak efficiencies. This is calculated for four peaks: the full (incident) energy peak, the single escape peak (incident energy - 0.511 MeV), the double escape peak (incident energy - 1.022 MeV) and the 0.511 MeV peak. Essentially, the efficiency of a peak is the number of counts in the peak (counts falling in the range `peak energy - DELTAE` $\leq$ `E` $\leq$ `peak energy + DELTAE`) minus the background near the peak (counts falling in the range `peak energy - 2*DELTAE` $\leq$ `E` $<$ `peak energy - DELTAE` or `peak energy + DELTAE` $<$ `E` $\leq$ `peak energy + 2*DELTAE` ) expressed as a fraction of the total energy in the pulse height distribution. Note that this analysis of peak efficiencies only makes sense for a monoenergetic incident beam.

**Restrictions**
When pulse height distributions are being scored, there are several restrictions on the variance reduction techniques which can be used. In particular, the particles weight cannot be changed inside the geometry past an initial weight change due to forcing (so, eg, bremsstrahlung splitting cannot be used, nor focing after the initial photon). In addition, if a phase space file is being used for input, ALL particles must have the same weight (= 1.0). These restrictions come about because, within each history, all particles must have the same weight, or else the scoring routines will be incorrect.

`IFULL= scatter fraction`
DOSRZnrc will output the total dose and the scatter dose. Scatter dose is defined as dose that can be traced back to photons that have been scattered in compton events and to photons that were created through relaxation processes after compton and photoelectric events. Note that this definition of scatter dose may not suit your particular problem, however it can be modified in the `AUSGAB` routine of DOSRZnrc.

### 3.5.2 `STATISTICAL ACCURACY SOUGHT`

If you supply a value for `STATISTICAL ACCURACY SOUGHT` other than zero, then DOSRZnrc will stop when the total dose in the region of maximum total dose has a percent uncertainty equal to `STATISTICAL ACCURACY SOUGHT`, provided that `NUMBER OF HISTORIES` (see section 2.10.1(page 38)) or `MAX CPU HOURS ALLOWED` (see section 2.10.3(page 39)) have not been reached first.

### 3.5.3 `SCORE KERMA` option

By setting `SCORE KERMA= yes` the user can output the kerma in a simulation. Kerma in a region is the total energy of charged particles set in motion by pair, compton or photoelectric events in that region. It also includes energy deposited in that region by electrons that aren't traceable back to pair, compton or photoelectric events (ie primary electrons). If the user chooses to score kerma and also has set `IFULL= scatter fraction`, then DOSRZnrc will also output the scatter kerma, which is the kerma due to scattered photons as defined in subsection 3.5.1(page 63).

## 3.6 Photon cross section enhancement (DOSRZnrc)

Cross section enhancement allows a user to increase the photon cross section of a material in an arbitrary region in the geometry by a factor $C_e$, and hence to increase the interaction density by that factor. This technique is useful when the goal of the simulation is to calculate energy deposition in a relatively small part of the geomtry (the original motivation for the implementation was the dose calculation in the thin sensitive regions of a dosimetric film placed in a big phantom).

Within the specified region, the cross section is enhanced by a factor $C_e$ and the position of the next interaction is determined.

The implementations is as follows: when an interaction is about to occur in a region with cross section enhancement, the incident photon is split into an interacting portion (fraction $1/C_e$) and a non-interacting portion (fraction $1 - 1/C_e$). All particles originating from the interaction carry the weight $w_0/C_e$, where $w_0$ is the weight of the original photon. Out of these particles all electrons are kept on the stack and transported, all photons (including relaxation photons, bremsstrahlung and annihilation photons from subsequent electron transport) are terminated with probability $1/C_e$ so that, if they survive, they have again the weight $w_0$. The unscattered portion of the incident photon is also terminated via Russian Roulette with probability $1 - 1/C_e$ making the weight of survivors $w_0$. In this way all electrons set in motion in the cross section enhancement region carry the weight $w_0/C_e$ and there are $C_e$ time more such electrons compared to a normal transport (without cross section enhancement). Note, however, that if an electron that was set in motion outside the cross section enhancement region enters that region, it will have a weight of $w_0$ and therefore increase the statistical fluctuations. Therefore, in order to use this method efficiently, it is a good idea to make the cross section enhancement region slightly larger than the region of interest so that no "fat" electrons can get into the volume of interest.

The inputs related to cross section enhancement are summarised below. The start and stop region can contain multiple numbers so as to define a specific region in an RZ geometry. The input is to be placed within the `:start variance reduction:` and `:stop variance reduction:` delimeters common for all RZ codes.

```
CS ENHANCEMENT FACTOR=       can scale the photon cross section
               by this factor in a specified set of regions.
               From 1 to 10,000. With a default of 200 if it is on at all.
CS ENHANCEMENT START REGION=
CS ENHANCEMENT STOP REGION=
               Photon cross section scaled in these defined sets of regions.
               From 2 to NREG. Defaults to region 1 which means no
               enhancement since this is outside the geometry.
```

Note that in the DOSRZnrc implementation the above input does not define $C_e$ directly. Instead, the input sets the desired number of interactions per g/cm$^2$, a definition that was found more convenient for our purposes. If we denote this number by $C$ and the photon

attenuation coefficient by $\mu$, the resulting cross section enhancement factor will be

$$C_e = \frac{C\rho}{\mu} \tag{9}$$

where $\rho$ is the mass density in the region. If C is selected so that $C_e \leq 1$ (eg if the attenuation coefficient is very large), cross section enhancement is turned off. This is exactly the desired behaviour: if the the photon already interacts at a very high rate due to its large attenuation coefficient, there is no need of an additional increase in the interaction density.

## 3.7 Plotting control

DOSRZnrc has a section of inputs to control plotting of dose vs depth/radius results. These inputs must be put between the delimiters `:start plot control:` and `:stop plot control:`. The inputs are:

```
  PLOTTING
         = Off          (0)   no plots or plot files to be prepared
         = On           (1)   plotting to be prepared or printed

 ONLY IF   PLOTTING= On
  LINE PRINTER OUTPUT
         = Off          (0)   don't plot in egslst file
         = On           (1)   do plot in egslst file

  EXTERNAL PLOTTER OUTPUT
         = Off          (0)   don't prepare plot files for xmgrace
         = On           (1)   prepare plot  files for xmgrace

  only if   EXTERNAL PLOTTER OUTPUT= On
  EXTERNAL PLOT TYPE
         = Point        (1)   point plot in xmgrace file
         = Histogram    (2)   histogram  plot in xmgrace file
         = Both         (3)   both point plot and histogram

  PLOT RADIAL REGION IX  (M)  radial regions to plot vs depth
                              (= 0 for no plots)

  PLOT PLANAR REGION IZ  (M)  planar slab numbers to plot vs radius
                              (= 0 for no plots)
```

You must have `PLOTTING= On` if you want to get any plots at all.

If you are plotting dose, then you must select the cylinders and/or slabs in your geometry for which you want to plot the dose. Cylinders are selected using the `PLOT RADIAL REGION IX` input and are numbered from the inside out. For example, if you just want to plot dose on the central axis you would input `PLOT RADIAL REGION IX= 1`, if you want to plot dose on the central axis and also the next cylinder out you would input `PLOT RADIAL REGION`

`IX= 1,2`, and so on. Doses in cylinders are plotted as dose vs. depth and are all written to the file `inputfile_dd.plotdat`. Slabs are selected using the `PLOT PLANAR REGION IZ` input and are numbered from the top (min. Z) down. So if you want to plot dose in, say, the topmost slab and also in slab number 10 of your geometry, you would input `PLOT PLANAR REGION IZ= 1,10`. Doses in slabs are plotted as dose vs. radius and are all written to the file `inputfile_rad.plotdat`.

If you select `LINE PRINTER OUTPUT= On`, then you will obtain plots of total ("T") and total-stopper ("S") dose vs. depth/radius in the `.egslst` file for the cylinders/slabs you have selected.

# 4 FLURZnrc

## 4.1 Introduction

FLURZnrc calculates the fluence of different particles in an RZ geometry. The fluence in each region is calculated, differential in energy, as the total pathlength in a given energy bin divided by the volume of the region. This has been formally shown to be equivalent to the fluence averaged over the volume[22, 23]. On a given charged particle step, the energy of the particle may be in more than one energy bin. The pathlength is assigned to the various energy bins using the approximation that the restricted stopping power is constant during the step. This approximation is good for higher energy charged particles but is increasingly poor for low-energy particles. One way to overcome this approximation is to restrict the energy loss in any given charged particle step to a smaller fraction (*e.g.*,, `ESTEPE = 0.01`). In a study of 2 MeV electrons slowing down in water, the change in the fluence was less than 0.5% when using 20 keV energy bins.

There are a variety of outputs such as total fluence as a function of position, spectra in each region and spectra of primaries vs secondaries of various types. The geometry and source inputs are identical to DOSRZnrc (described above).

This code (or its ancestor FLURZ) has been used frequently in the literature, often in conjunction with DOSRZ (see, eg [24]).

## 4.2 Input/output control

I/O control input is delimited between `:start I/O control:`
and `:stop I/O control:`. In addition to the common I/O inputs described in section 2.9 FLURZnrc has the following I/O inputs which are discussed in more detail below:

```
PRINT FLUENCE SPECTRA
      = all          (0)  print all fluence spectra
      = specified    (2)  print spectra only for those regions
                          specified by 'LIST FLUENCE START REGION'
                          and 'LIST FLUENCE STOP REGION'.
      = none         (3)  no fluence spectra printed
```

```
 LIST FLUENCE START REGION    (only if  PRINT FLUENCE SPECTRA= specified)
                     (M)  Lower (starting) numbers defining the regions for
                          which spectra are to be printed in listing file.

 LIST FLUENCE STOP REGION    (only if  PRINT FLUENCE SPECTRA= specified)
                     (M)  Higher (final) numbers defining the regions for
                          which spectra are to be printed in listing file.
 IPRIMARY
       = total fluence             (0) score total fluence spectra  only

       = electron primaries        (1) score electron primaries
                                       separately. Include brem
                                       generated photons as primaries
       = include brem secondaries  (2) score electron primaries
                                       but include those generated by brem
                                       as secondaries
       = photon primaries          (3) primaries are all first generation
                                       photons,including brem.
                                       Secondaries include all scattered
                                       photons and annihilation photons.
       = electron secondaries      (4) Score electron secondaries.


 SLOTE      (R)  = 0.0  => read in energy bins for output,
                 = -999    set up $EBIN bins, top 10% linear for SPR calc
                 < 0       set up -SLOTE equal log bins
                 else   set up equal bins of SLOTE. If too many bins
                        are requested, SLOTE is doubled until the number of
                        bins needed to cover the spectrum is <= $EBIN

-------------------------------------------------------------------------------
 (if SLOTE=0.0)
 TOPS OF ENERGY BINS (M)  tops of output bins in MeV
                          starting with the lowest,
                          end with value < or = last value
```

### 4.2.1 PRINT FLUENCE SPECTRA options

The user has control of which fluence spectra get output to the .egslst file using the PRINT FLUENCE SPECTRA input. If the user selects PRINT FLUENCE SPECTRA= all, then total fluence spectra (as well as any primary or secondary fluence spectra selected using IPRIMARY) for electrons, photons, positrons and charged particles are output for all regions in the geometry. This can lead to a huge quantity of output. The user can specify that fluence spectra be output only for selected regions using PRINT FLUENCE SPECTRA= specified and then LIST FLUENCE START REGION and LIST FLUENCE STOP REGION to specify the regions

for which the spectra are to be output. Alternatively, if the user is only going to look at the fluence spectra graphically (using a plotting program such as `xmgrace` together with the output to the .plotdat file) then the user can set `PRINT FLUENCE SPECTRA= none` to prevent an unnecessarily large `.egslst` file.

The input parameter `SLOTE` is used to control the energy binning in all fluence spectra. As indicated above, if `SLOTE` $> 0.0$, then equal energy bins of width `SLOTE` are used to cover the entire energy range of the fluence spectra. If `SLOTE= 0`, then the user supplies the tops of the energy bins using the `TOPS OF ENERGY BINS` input. If `SLOTE` $< 0$, then `-SLOTE` logarithmically-spaced energy bins are set up to cover the entire energy range. Finally, if `SLOTE= -999`, FLURZnrc will use `$EBIN` (macro defining the maximum number of energy bins possible–adjustable in `flurznrc.mortran`) energy bins to cover the energy range with 90% of the energy range being covered by logarithmically-spaced bins and the top 10% of the energy range being covered by linearly-spaced bins. This is designed for calculations of stopping-power ratios (see ref[24]).

### 4.2.2 `IPRIMARY` options

Using the `IPRIMARY` input, the user can choose to output primary/secondary photon spectra based on a number of different criteria.

The following two options are designed for use with incident beams of charged particles.

If `IPRIMARY= electron primaries`, then, in addition to the total fluence spectra for each particle type, FLURZnrc will output primary fluence spectra for each particle type that exclude knock-on electrons from Moller interactions and also exclude any secondary particles that these electrons may set in motion. Thus, this definition of electron primaries includes electrons set in motion by bremsstrahlung photons which were generated by electrons set in motion by primary photons..

The `IPRIMARY= include bremsstrahlung secondaries` is similar to the "electron primaries" option, only now the primary fluence spectra will also exclude bremsstrahlung photons and any secondary particles that they set in motion.

The following option was designed for use with an incident photon beam.

If `IPRIMARY= photon primaries`, then FLURZnrc will output primary fluence spectra for all particles that exclude photons scattered in compton and Rayleigh events, e-/e+ pairs created in pair production events, electrons set in motion by compton and photoelectric events, any relaxation particles created after compton or photoelectric events, and any higher-order particles set in motion by these excluded particles. Note that this definition means that no charged particles are included as primaries.

If the user selects `IPRIMARY= electron secondaries`, then FLURZnrc outputs secondary fluence spectra for all particles that include knock-on electrons from Moller events and any secondary particles that these electrons may set in motion. Note that in this definition of electron secondaries, electrons created by bremsstrahlung photons are considered primaries.

## 4.3 Monte Carlo inputs

FLURZnrc has no other Monte Carlo inputs than those that are common for all user codes. These common Monte Carlo inputs are described in section 2.10(page 38).

## 4.4 Plotting control

FLURZnrc has two distinct types of plotting outputs. One class of plots gives integral fluence vs position plots in various ways (vs depth, vs radius). The code also outputs fluence spectra in specified regions.

The user controls the plotting using the following input parameters that must appear between the `:start plot control:` and `:stop plot control:` delimiters:

```
 PLOTTING
        = Off          (0)   no plots or plot files to be prepared
        = On           (1)   plotting to be prepared or printed


ONLY IF   PLOTTING= On
        Note that most of the following affects both fluence and spectral
        plots.
EXTERNAL PLOT TYPE
        = Point        (1)   point plot on external plotter
        = Histogram    (2)   histogram on external plotter
        = Both         (3)   both point plot and histogram


DRAW FLUENCE PLOTS
        = none        (1,0)  plot total fluence (as a minimum)
        = all         (1,1)  plot total and primaries
        = primaries   (0,1)  plot primaries only
        = total       (1,0)  plot total fluence (the minimum)
                             [IPLPHB]


PLOTS FOR ELECTRONS
        = Off          (0)   don't generate plots for electrons
        = On           (1)   generate plots for electrons

PLOTS FOR PHOTONS
        = Off          (0)   don't generate plots for photons
        = On           (1)   generate plots for photons

PLOTS FOR POSITRONS
        = Off          (0)   don't generate plots for positrons
        = On           (1)   generate plots for positrons
```

```
PLOTS FOR E- AND E+
        = Off          (0)   don't generate plots for e- and e+
        = On           (1)   generate plots for e- and e+

START SPECTRAL PLOT IN REGION
                     (M)  lower (starting) numbers defining the regions for
                          which spectra are to be printed in .spectra file.

STOP SPECTRAL PLOT IN REGION
                     (M)  higher (final) numbers defining the regions for
                          which spectra are to be printed in .spectra file.

 PLOT RADIAL REGION IX  (M)  radial plane numbers to plot integral
                             fluence (= 0 for no plots)

 PLOT PLANAR REGION IZ  (M)  planar slab numbers to plot integral fluence
                             (= 0 for no plots)
```

The user must select `PLOTTING= On` to obtain any plots at all.

### 4.4.1 Plotting fluence (`.plotdat`)

Fluence plots are output to a `.plotdat` file in which fluence vs depth/radius is formatted for immediate plotting using `xmgrace` or similar plotting program.

Use `PLOT RADIAL REGION IX` to select the cylinders to plot fluence vs. depth in and `PLOT PLANAR REGION IZ` to select the slabs to plot fluence vs radius in. Use of these inputs is similar to DOSRZnrc's input (see section 3.7(page 65)).

Using `DRAW FLUENCE PLOTS` the user can then select whether to plot only the total fluence, the total fluence and any primaries/secondaries selected using the `IPRIMARY` input (see section 4.2.2), or just the primaries/secondaries. Note that, as a minimum, total fluence gets output (ie even when `DRAW FLUENCE PLOTS= none`).

Fluence data can be plotted for photons (`PLOTS FOR PHOTONS= on`), electrons (`PLOTS FOR ELECTRONS= on`) and positrons (`PLOTS FOR POSITRONS= on`). The input for charged particles, `PLOTS FOR E- AND E+`, is only valid for for fluence spectra plots (see section 4.4.2).

Finally, the user can choose to plot fluence histograms, point plots, or both on the same plot using the `EXTERNAL PLOT TYPE` input.

If you are using `xmgrace` to examine the plots, each curve will be labelled with its cylinder/slab number ("radial zone"/"planar zone"), the particle charge ("IQ"), and whether this is the total fluence ("IP=1") or primary/secondary fluence ("IP=2").

Note that all fluence data gets put into the same `.plotdat` file, which may lead to confusion if you are plotting both fluence vs depth (in cylinders) and fluence vs radius (in slabs) data.

### 4.4.2 Plotting spectra (.spectra)

If you have selected PLOTTING= On, then you can also obtain fluence spectra plots. Fluence vs energy data are output to a .spectra file which is in a format that can be viewed using xmgrace or similar plotting package. The energy resolution of these plots is determined by the SLOTE input explained in section 4.2.1(page 67).

Use the START SPECTRAL PLOT IN REGION and STOP SPECTRAL PLOT IN REGION inputs to define a range (or ranges) of regions for which you want fluence spectra. For each region in the range, fluence vs. energy data will be output. Thus, if you input

```
START SPECTRAL PLOT IN REGION= 2, 43
TOP SPECTRAL PLOT IN REGION= 3, 45
```

you will get fluence spectra for regions 2, 3, 43, 44, 45.

Note that PLOT RADIAL REGION IX and PLOT PLANAR REGION IZ are for fluence vs depth or radius plots only (see section 4.4.1 (page 70)), not fluence spectra.

Using the input DRAW FLUENCE PLOTS, you can plot the total fluence spectra, total spectra and the spectra of any primary/secondaries that you have selected or just the primary/secondary spectra. As a minimum, the total fluence spectra are output.

You can also select which particles you want to output fluence spectra for using the PLOTS FOR PHOTONS, PLOTS FOR ELECTRONS, PLOTS FOR POSITRONS and PLOTS FOR E- AND E+ inputs. Note that all of these inputs, except for PLOTS FOR E- AND E+ are also available for fluence vs depth/radius plots.

Finally, similar to fluence vs. depth/radius you can plot histograms, points or both using the EXTERNAL PLOT TYPE input.

Note that output of the .spectra file and the .plotdat file are not mutually exclusive. If you do choose to output both at the same time, then you must make sure that the settings of DRAW FLUENCE PLOTS, PLOTS FOR PHOTONS, PLOTS FOR ELECTRONS, PLOTS FOR POSITRONS and EXTERNAL PLOT TYPE, which affect both spectra and fluence vs depth/radius plots, include all the information you want from both sets of plots.

# 5 SPRRZnrc

## 5.1 Introduction

This code calculates Spencer-Attix mass restricted collision stopping-power ratios in each region in an RZ geometry. It uses an on-the-fly technique for scoring which has been described briefly in ref[20] and shown to get the same answers as the more traditional methods of calculating the fluence spectra as a first step, eg see ref[24]. These calculations have been verified against calculations using other codes and been shown to be in good agreement(see ref[24, 20]).

## 5.2 How stopping-power ratios are calculated

The standard definition of Spencer-Attix mass restricted collision stopping-power ratios is given by[25, 26]:

$$\left(\frac{\overline{L}}{\rho}\right)_{\mathrm{g}}^{\mathrm{m}} = \frac{\int_{\Delta}^{E_{max}} \Phi_{\mathrm{T}} \left(\frac{L(\Delta)}{\rho}\right)_m dE + TE_m}{\int_{\Delta}^{E_{max}} \Phi_{\mathrm{T}} \left(\frac{L(\Delta)}{\rho}\right)_g dE + TE_g} \tag{10}$$

where $\Phi_{\mathrm{T}}$ is the electron fluence spectrum at energy E, $\left(\frac{L(\Delta)}{\rho}\right)_{med}$ is the restricted mass collision stopping power of medium *med*, TE is a term to account for the 5 to 10% of the dose from track-ends (i.e. electrons whose energy falls below $\Delta$), $\Delta$ is the lowest energy for which secondary electrons are considered part of the electron spectrum (all secondaries below this are considered as absorbed on the spot and included in the restricted stopping power $\left(\frac{L(\Delta)}{\rho}\right)_{med}$). The track-end term corresponds to the total energy deposition by particles falling below $\Delta$ and is given by $\Phi_{\mathrm{T}}(\Delta)$ $\left(\frac{S(\Delta)}{\rho}\right)_{med}$ $\Delta$ [26, 27] (note that at $\Delta$, the restricted and unrestricted stopping powers are the same). The stopping-power ratio can be thought of as the ratio of the energy deposited in two media which have the same electron spectra.

In "traditional" Monte Carlo calculations of the stopping-power ratio, the fluence spectra in the medium without a cavity was scored using a fluence scoring code. The integral above was then evaluated off line. This can lead to huge quantities of data, especially if one wanted the stopping power as a function of depth in a medium. The present code was developed originally to be more convenient, and to avoid the necessity of manipulating large numbers of spectra. This approach also avoids issues about binning artifacts in the calculations since the fluence spectra are never binned. On the other hand, it also introduces some difficult issues about how to handle the low-energy stoppers. This is discussed somewhat below and certain implications of this issue have been discussed in some detail by Borg et al[28]. These difficulties actually exist when calculating electron spectra as a first step as well, but are more conveniently ignored in that case.

The basic approach of the SPRRZnrc code is to score the total dose deposited in the two different media, as represented by the numerator and denominator in equation 10 but for a calculation in which the cavity is filled with the transport medium, not the detector medium. The energy deposition can be thought of as having 4 distinct modes as shown in figure 2.

The dose delivered by the $\alpha$ events in figure 2 is simple to analyze. In the numerator we just sum the actual energy deposition. In the denominator we sum the energy deposition times the ratio of restricted stopping powers at the mid-point energy of the step, i.e.

$$EDEP \frac{\left(\frac{L(\mathrm{Emid})}{\rho}\right)_g}{\left(\frac{L(\mathrm{Emid})}{\rho}\right)_m} \tag{11}$$

This gives how much energy would be deposited in medium $g$ instead of medium $m$.

The $\beta$ events are not scored at all, except in an evaluation of the total dose. These events correspond to electrons or photons being created in the cavity region below the respective transport cut-offs. It is arguable how to deal with these events, but in traditional calculations

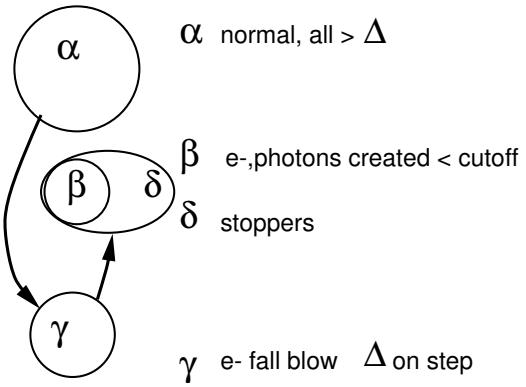


Figure 2: Modes of energy deposition considered in SPRRZnrc. $\alpha$ events are those in which energy is deposited by electrons in a step with the energy entirely above $\Delta$. $\gamma$ events are those in which the electron starts a step with its energy greater than $\Delta$ and ends with an energy below $\Delta$. The $\delta$ events are all those events in which an electron or photon are being terminated because they are below the cutoffs AE or AP. This includes a subset of $\beta$ events formed by electrons and photons which are created with their energy initially below AE or AP.

starting from electron spectra they were either ignored or lumped in with the stoppers. This issue has been discussed in Borg et al, and there is no clear solution at this time[28]. However, the fraction of the dose contributed in the cavity region from these events is output by SPRRZnrc and found to be very small for electron beams or for photon beams at $^{60}$Co energies and higher. This fact makes the problem academic in most situations. The problem becomes serious for low-energy photon beams, but here the application of Spencer-Attix cavity theory is also suspect[28].

The $\delta$ or stopper events which are not $\beta$ events, are scored as part of the track-end term in eqn(10). This is done by scoring the natural energy deposition in the numerator and the same energy deposition multiplied by the ratio of the unrestricted stopping powers at $\Delta$ (which are equal to the restricted stopping powers), i.e.:

$$EDEP\frac{\left(\frac{S(\Delta)}{\rho}\right)_g}{\left(\frac{S(\Delta)}{\rho}\right)_m}. \tag{12}$$

Note that this does not merely correspond to the energy deposition in the second medium, because for a stopper, the energy deposition would be the same in both media (it just deposits all of its energy which is the same in both cases). The track-end term in eqn(10) is derived to take into account that the number of stoppers in each medium will differ because the fluence of particles stopping in each medium will differ and this number of stoppers is proportional to the stopping power.

The $\gamma$ events, those particles which cross $\Delta$ during their step are scored by treating the step as having two components. The component with energy above $\Delta$ is treated as if it were an $\alpha$ event and the component of the energy deposited below $\Delta$ is treated as a $\delta$ event.

The SPRRZnrc program scores 3 different doses: the total dose; dose including everything except the $\beta$ component (stoppers created below $\Delta$)[IT=1]; dose from $\alpha$ plus $\gamma$ only [IT=3].

Table 4: Energy deposition classes and their components

| IT value | included events |
|---|---|
| 1 | $\alpha + \gamma + (\delta - \beta)$ |
| 3 | $\alpha + \gamma$ |
| total | $\alpha + \gamma + \delta$ |

The IT=2 and IT=4 components correspond to the IT=1 and IT=3 components but scored in the $g$ material as outlined above. The code then outputs: the total dose; the fraction of the total dose due to included stoppers (IT=1 − IT=3)/total; and the fraction of the total dose due to excluded stoppers (total− IT=1)/total.

The IT=2 dose component is the same as the IT=1 dose component except as modified to represent the dose in the detector medium as described above. The IT=4 component similarly corresponds to the IT=3 component, i.e. the dose less the actual stoppers but including the crossers.

The stopping-power ratios are calculated as the IT=1 dose component divided by the IT=2 dose component (strictly the scored energy depositions divided by the respective densities are used). The stopping-power ratio less the stoppers is calculated by taking IT=3 divided by IT=4.

The code outputs he two different stopping-power ratios to demonstrate that the inclusion of the stoppers has only a small effect on the overall stopping-power ratio, which is a good thing since the treatment of the stoppers is somewhat arbitrary. However, it should be pointed out that the $\gamma$ events are not classified as stoppers but in fact they do contain some element of the stoppers dose since steps are not stopped at $\Delta$, but rather at some energy slightly less than $\Delta$.

## 5.3 Input/output control

I/O control input is delimited between `:start I/O control:`
and `:stop I/O control:`. Most I/O control input for SPRRZnrc is common to all user codes and is described in section 2.9(page 35). However, the `SPR OUTPUT` control is unique to SPRRZnrc and you input it as follows:

```
  SPR OUTPUT
        = regions          (0)  Specify stopping power ratio output by
                                regions (no .plotdat file will be generated)
        = slabs/cylinders (1)  Specify stopping power ratio output by slabs
                                & cylinders (.plotdat file is generated)
*****************************************************************************

  IF SPR OUTPUT= regions

  SPR START REGION    (M)  region numbers in which to start scoring stopping
                            power ratios
```

```
  SPR STOP REGION    (M)  region numbers in which to stop scoring stopping
                          power ratios

**************************************************************************

  IF SPR OUTPUT= slabs/cylinders

  SPR IN CYLINDER IX  (M)  Cylinder numbers for which to output
                           stopping power ratios (= 0 for no output)

  SPR IN SLAB IZ      (M)  planar slab numbers for which to output
                           stopping power ratios (= 0 for no output)

**************************************************************************
```

### 5.3.1 `SPR OUTPUT` options

`SPR OUTPUT` is used to determine how stopping power ratios are output. If electron range rejection is off, then stopping power ratios in all regions are output to the `.egslst` file. If electron range rejection is on, then stopping power ratios are zeroed in the `.egslst` file except in regions specified using `SPR START REGION` and `SPR STOP REGION` (if `SPR OUTPUT= regions`) or in slabs/cylinders specified using `SPR IN CYLINDER IX` and `SPR IN SLAB IZ` (if `SPR OUTPUT= slabs/cylinders`). In addition, electron range rejection is automatically turned off in the regions/slabs/cylinders you have selected for output so that the stopping power ratios will be meaningful. If you are using the `SPR OUTPUT= slabs/cylinders` option, then you will also get a `inputfile_dd.plotdat` file which contains the stopping power ratios (and doses) in the selected slabs and a `inputfile_rad.plotdat` file containing stopping power ratios (and doses) in the selected cylinders. This files are in a format that can be plotted with `xmgrace` or other plotting program.

## 5.4 Monte Carlo control

Monte Carlo control input is delimited between `:start Monte Carlo inputs:` and `:stop Monte Carlo inputs:`. In addition to the Monte Carlo inputs common to all user codes (see section 2.10(page 38)), SPRRZnrc has the following Monte Carlo input:

```
  PHOTON REGENERATION         (C)  yes => primary photons are regenerated
                                          after they interact and scattered
                                          photons are thrown away.
                                   no (default) => full calculation
```

### 5.4.1 PHOTON REGENERATION option

The photon regeneration option is used to calculate the stopping power ratios for electrons resulting from an unattenuated and unscattered photon beam. If `PHOTON REGENERATION= yes`, then, prior to a pair production, compton, photoelectric or Rayleigh event, the properties of the photon about to interact are saved. After the interaction, any scattered photons or photons resulting from relaxation process are discarded and (once all secondary electrons have been transported) transport reverts to the duplicate photon that was saved just before the interaction. In addition, photons resulting from bremsstrahlung events and positron annihilation events are eliminated on the spot.

This option is to be used when calculating stopping-power ratios for use in air kerma cavity ion chamber standards since the basic theory makes this assumption. This makes the calculated stopping-power ratio independent of the details of the geometry as long as there is full buildup. This is discussed in detail by Borg et al[28]. This option should not be used when calculating stopping-power ratios in a phantom since in that case you want the effects of scatter and attenuation to be taken into effect.

# 6 CAVRZnrc

## 6.1 Introduction

CAVRZnrc calculates various factors of interest when using cavity ion chambers such as $A_{att}$ and $A_{scat}$ and $A_{wall}$. It has been described in detail in various publications[29, 30, 31, 32] and shown to produce results in good agreement with standard theory[28].

## 6.2 Cavity inputs

CAVRZnrc requires an extra set of inputs defining the cavity region. These inputs must appear between the delimiters `:start cavity inputs:` and `:stop cavity inputs:`.

If the user has input the radial geometry using `METHOD OF INPUT= individual` or `METHOD OF INPUT= groups` (see section 2.5.1(page 12)), then the following inputs must appear between the cavity input delimiters:

```
NUMBER OF CAVITY REGIONS (I)   number of geometrical zoneS
                               comprising the cavity.

REGION NUMBERS OF THE CAVITY  (M)
                               the array of these zones
                               (the cavity region numbers)
```

Thus, the user defines the cavity in terms of region numbers within the geometry.

Alternatively, CAVRZnrc offers another method for entering the geometry in which the geometry is automatically defined based on cavity information specified by the user. In this

case, only `METHOD OF INPUT= cavity information` needs to be entered between the `:start geometrical inputs:` and `:stop geometrical inputs:` delimiters. Then, between the cavity input delimiters, the following inputs must be supplied:

```
WALL THICKNESS      (R)   thickness of the chamber walls (cms)
                          (defaults to 0.273)

CAVITY RADIUS       (R)   outer radius of the cavity (cms)

CAVITY LENGTH       (R)   length of the cavity (cms) (defaults to 0.2)

ELECTRODE RADIUS    (R)   radius of the electrode (defaults to 0.)

WALL MATERIAL       (C)   wall material

only if   ELECTRODE RADIUS > 0.0
ELECTRODE MATERIAL  (C)   electrode material
```

CAVRZnrc creates a simple 3-cylinder (`RCYL(1)=ELECTRODE RADIUS, RCYL(2)= CAVITY RADIUS, RCYL(3)= CAVITY RADIUS + WALL THICKNESS`), 3-slab (`ZPLANE(1)=0, ZPLANE(2)=WALL THICKNESS, ZPLANE(3)=WALL THICKNESS + CAVITY LENGTH, ZPLANE(4)=2*WALL THICKNESS + CAVITY LENGTH`) geometry based on these inputs. The material in the cavity is assumed to be AIR. This option was useful for early calculations but is not adequate for chambers in which we want to include much detail.

## 6.3 Input/output control

As with the other user codes, I/O control inputs must appear within the delimiters `:start I/O control:` and `:stop I/O control:`. In addition to I/O controls that are common to all user codes (see section 2.9(page 35)), CAVRZnrc has the following inputs:

```
STORE INITIAL RANDOM NUMBERS
      = no          (0)  do not store initial random numbers
      = last        (1)  store initial random number for last history
      = all deposited (2)store the initial random number for all
                         that deposit energy in the cavity
      = all         (3)  store all the initial random numbers

OUTPUT OPTIONS
      = short              (0)  short output -just the cavity summary
                                and the dose grid.
      = cavity details     (1)  above plus details for each cavity zone
```

The `STORE INITIAL RANDOM NUMBERS` input has been included here because CAVRZnrc has one option, `STORE INITIAL RANDOM NUMBERS= all deposited`, that is not included in the other user codes (see section 2.9.2(page 35)). With this option, the initial random numbers from only those histories that end up depositing energy in the cavity region are stored

in the `.egsrns` file. Then, if the run is restarted with `IRESTART= start-RNS` (see section 2.9.3(page 36)), all histories will end up depositing energy in the cavity region.

If the user chooses `OUTPUT OPTIONS= short`, then dose and correction factors will only be output for the cavity as a whole. If `OUTPUT OPTIONS= cavity details`, then dose and correction factors will be output for the cavity as a whole and for each region that makes up the cavity.

## 6.4 Monte Carlo control

Monte Carlo control input is delimited between `:start Monte Carlo inputs:` and `:stop Monte Carlo inputs:`. In addition to Monte Carlo inputs that are common to all user codes (see section 2.10(page 38)), CAVRZnrc had the following Monte Carlo inputs:

```
IFULL
       = dose and stoppers     (0) just calculate total dose
       = Aatt and Ascat        (1) Above plus Aatt, Ascat
       = Ap                    (2) Above plus Ap as well (option
                                   currently disabled)
       = Afl and <s>g/w        (3) Above plus Afl and <s>g,w as well
                                   (option currently disabled)

STATISTICAL ACCURACY SOUGHT    (R) % statistical accuracy of the total
                                   dose in the peak region that is
                                   sought The program executes until this
                                   accuracy is obtained or the CPU time
                                   runs out.
PHOTON REGENERATION
       = yes (1) the calculation is performed with regeneration
                         of the parent photon after they have
                         interacted. A typical setting when FANO
                         conditions are examined.
       = no (0)  a normal calculation.
       = no electrons from wall (ifano = 2) secondary electrons from
                         interactions in the cavity wall are immediately
                         eliminated.  Photons are not regenerated.
                         [IFANO]
```

### 6.4.1 `IFULL= dose and stoppers` option

If `IFULL= dose and stoppers`, then CAVRZnrc will output the total dose in the cavity and, if `OUTPUT OPTIONS= cavity details`, in each region making up the cavity to the `.egslst` file.

### 6.4.2 `IFULL= Aatt and Ascat` option

The methods used to calculate the various correction factors have been described in the literature[29, 30, 33, 31].

If `IFULL= Aatt and Ascat`, then CAVRZnrc will output the total dose, $A_{att}$, $A_{scat}$ and $A_{wall}$ in the cavity and, if `OUTPUT OPTIONS= cavity details`, in each region of the cavity to the `.egslst` file. The listing files also include $K_{wall} = 1./A_{wall}$ (etc).

The scatter correction factor, $A_{scat}$, is defined as the ratio of the total energy deposited in the cavity to the energy deposited by electrons generated by primary photon interactions [33]. In CAVRZnrc, photons are flagged as secondary if they have been scattered in compton, or Rayleigh events, generated by bremsstrahlung or positron annihilation events, generated by atomic relaxations after compton or photoelectric events, or if their energy is deposited locally because they have energy < N-shell energy in a photoelectric event. Once CAVRZnrc has totalled the energy deposited in the cavity by electrons generated by primary photons ($ECAV_{prim}$), and the energy deposited in the cavity by electrons generated by photons flagged as secondary ($ECAV_{sec}$), $A_{scat}$ is calculated using the equation:

$$A_{scat} = 1 + \frac{ECAV_{sec}}{ECAV_{prim}} \tag{13}$$

### 6.4.3 `STATISTICAL ACCURACY SOUGHT`

If you input a value for `STATISTICAL ACCURACY SOUGHT` other than zero, then CAVRZnrc will stop when the percent uncertainty on the total dose in the cavity volume (all cavity regions combined) is equal to `STATISTICAL ACCURACY SOUGHT` provided that `NUMBER OF HISTORIES` (see section 2.10.1(page 38)) or `MAX CPU HOURS ALLOWED` (see section 2.10.3 (page 39)) have not been reached first.

### 6.4.4 `PHOTON REGENERATION` options

CAVRZnrc offers two photon regeneration options. If the user selects `PHOTON REGENERATION= yes`, then photon regeneration is similar to that in SPRRZnrc (see section 5.4.1(page 76)). Unlike SPRRZnrc, where it is required for proper stopping power ratio calculations as used in primary air-kerma standards, the purpose of this option in CAVRZnrc is mainly for theoretical benchmark calculations (*e.g* testing for artefacts under Fano conditions). An additional use could be for an independent verification of $A_{wall}$: one runs simulations with `PHOTON REGENERATION= ON` and `PHOTON REGENERATION= OFF`, the ratio of the two doses is per definition $A_{wall}$. This is however not very efficient and a better way to accomplish this task is to use the cross section enhancement or photon splitting options described below.

The second regeneration option in CAVRZnrc is `PHOTON REGENERATION= no electrons from wall`. With this option, charged particles resulting from pair production, compton and photoelectric events are eliminated provided that the interaction did not take place inside the cavity. This is a hack that has been used to study the dose fraction from photon interactions in the cavity.

## 6.5 CAVRZnrc variance reduction techniques

### 6.5.1 Photon cross section enhancement

The cross section enhancement technique in CAVRZnrc is similar to the one implemented in DOSRZnrc (see section 3.6 page 64) but in CAVRZnrc it is applied globally in the entire geometry and the value of $C_e$ is input directly (as opposed to C as input in the DOSRZnrc case). Cross section enhancement in CAVRZnrc can be turned on by including the following line in the input file:

```
CS ENHANCEMENT FACTOR=  some real number [cs_enhance]
```

If the input is missing or less than unity, there will be no effect. But if the enhancement factor is set to greater than unity, the effect is dramatic: all other user input concerning photon forcing, splitting, exponential transform, etc., is ignored. In addition, the calculation result always corresponds to the `IFULL= Aatt and Ascat` option, no matter what the user requested (but only $A_{wall}$ is calculated, not the individual $A_{scat}$ and $A_{att}$, see section 6.4.2). In addition, all scoring is done using proper history-by-history statistics using the common block `score1`. The drawback is that dose and $A_{wall}$ are calculated for the whole cavity and not on a region-by-region basis as under normal CAVRZnrc operation.

The following text gives a brief description of the differences to the DOSRZnrc implementation: The motivation behind the implementation of cross section enhancement in CAVRZnrc was the desire to have an independent calculation technique for $A_{wall}$ that is not too inefficient compared to the unweighting technique. Indeed, $A_{wall}$ can be calculated by running two separate CAVRZnrc simulations, one with normal transport and one with attenuation and scatter removed via the `photon regeneration= on` option. The ratio of the cavity dose from the former to the dose from the latter calculation is by definition $A_{wall}$. Because both calculations are uncorrelated, their uncertainties add in quadrature and so, the uncertainty on $A_{wall}$ is larger than the individual dose uncertainties. The purpose of the cross section enhancement implementation in CAVRZnrc is to make the two necessary dose calculations at once and thus reduce the uncertainty of $A_{wall}$ because of the strong correlation between the "normal" dose and the dose with attenuation and scatter removed. To accomplish this task, scattered photons are killed as in DOSRZnrc with probability $1/C_e$. If they survive, they are marked as scattered by setting their `latch` variable to 3. Unlike in DOSRZnrc, the unscattered portion of primary photons is always kept on the stack and transported. However, these non-scattered fractions of primary photons are marked as attenuated primary photons (`latch=2`) with probability $1 - 1/C_e$ and therefore their descendents only contribute to the dose with attenuation and scatter removed. In addition, scatter, bremsstrahlung and annihilation from `latch=2` particles are immediately removed from the stack. It is then clear that `latch=0,2` electrons contribute to the dose with attenuation and scatter removed, `latch=0,3` electrons to the normal dose.

### 6.5.2 Photon splitting

An additional variance reduction scheme offered in CAVRZnrc is the photon splitting technique. Input that turns on photon splitting must appear between the `:start variance reduction:` and `:stop variance reduction:` delimiters and is:

```
PHOTON SPLITTING=    (I)    Number of times to split a photon
                            If missing or < 2  => normal transport
                            If >= 2 (allowed only for ifull= dose and
                            stoppers or = Aatt and Ascat), the macro
                            $SELECT-PHOTON-MFP essentially replaces the
                            entire PHOTON routine.
                            [n_split]
```

This technique is borrowed from Ref. [34] where it was shown to increase the efficiency of external photon beam calculations for radiotherapy by up to a factor of 5. The increase in CAVRZnrc is not so dramatic, nevertheless an increase in the efficiency of cavity dose calculations of up to a factor of 3 compared to using photon forcing has been observed.

This option is only available with `IFULL= dose and stoppers or =Aatt and Ascat`. It is also possible to use the `ifano` option (only if `IFULL=0`). Note that with photon splitting on, all scoring is done using proper history-by-history statistics using the common block `score1`. The drawback is that dose (and $A_{wall}$ if requested) are calculated for the whole scoring cavity and not on a region-by-region basis as under normal CAVRZnrc operation.

The algorithm works as follows: each photon that is to be transported is split into `n_split` photons with weights $w_0$/`n_split` ($w_0$ is the original photon weight). The number of mean-free-paths $\lambda_i$ to the next interaction of the $i$'th such photon is sampled from

$$\lambda_i = -\ln\left[1 - \frac{\xi + i - 1}{\texttt{n\_split}}\right] \tag{14}$$

where $i$ runs from 1 to `n_split` and where $\xi$ is a random number. This forces a uniform distribution of interaction sites. In addition we have $\lambda_{i+1} > \lambda_i$ and therefore only transport from $\lambda_i$ to $\lambda_{i+1}$ is needed to get to the interaction site of the $i+1$'st photon from the interaction site of the $i$'th photon. When one of the split-photons interacts, all resulting scattered photons are killed with probability 1/`n_split` and marked as scattered if they survive (`latch=3`). If `IFULL= Aatt and Ascat` or `photon regeneration= on`, the original photon is re-created at each interaction site with probability 1/`n_split` and marked as a regenerated photon (`latch=2`). As for the cross section enhancement technique, `latch=0,3` particles contribute to the normal dose, `latch=0,2` particles to the dose with attenuation and scatter removed. The ratio of the two is $A_{wall}$ and so, photon splitting is a third independent technique for calculating this quantity.

A rule of thumb for good efficiency is to use

$$n\_split \geq \frac{N_o}{1. - e^{-\lambda}} \tag{15}$$

where $\lambda$ is approximately the number of photon mean free paths in the geometry of interest and $N_o \geq 5$. For $^{60}$Co, $\lambda$ is about 0.06 for 1 g/cm$^2$ of graphite and so $n\_split$ should be $\geq 80$.

# 7 Spherical user codes

## 7.1 Introduction

Since 2003, the EGSnrc distribution includes a pair of spherical geometry user codes. CAVSPHnrc is the spherical analogue of CAVRZnrc, designed for ion chamber calculations, and has been used extensively for this purpose (see, *eg.*, references[35, 36]). The other code, EDKnrc, was derived from SCASPH, an EGS4 user code for the calculation of mono-energetic energy deposition kernels[37]. EDKnrc has been extended to allow the use of both monoenergetic and polyenergetic sources.

Both user codes share most of the common features of the RZ user codes excluding geometry and source types. We will describe these two in the following subsections and the user is refered to section 2 for information on the common input blocks of these codes.

## 7.2 Geometry and Material Inputs

### 7.2.1 Geometrical input: spheres and cones

The geometrical regions subtended by concentric spheres and cones originating at the common center of the spheres are shown in figure 3. NR represents the number of spheres and NC the number of cones. In what follows we explain the input specification of the geometry.

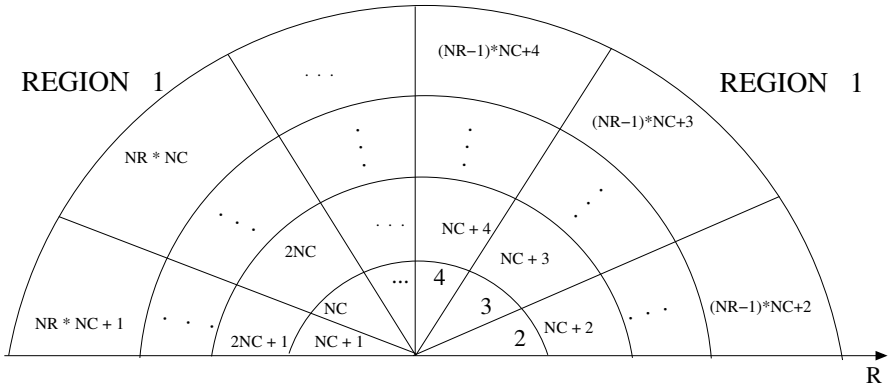


Figure 3: Region numbering scheme for the spherical user codes. Region number 1 is always outside the geometry. The first region (2) is defined by the innermost sphere and the cone with the smallest opening angle. `NR` is the number of radial zones = # radii and `NC` = number of cones (0 for purely spherical geometry).

As in the RZ codes, the geometry inputs are delimited by the strings `:start geometrical inputs:` and `:stop geometrical inputs:`. The meaning of the inputs depends on the entries for `NUMBER OF CONES` and `NUMBER OF SPHERES`. If a single value is input, then the user is expected to input the individual corresponding radii or angles. If multiple values are given for `NUMBER OF CONES` and/or `NUMBER OF SPHERES`, the user is expected to put in groups of equal angles and/or radii. If, for instance, several entries are made for the number of angles, *i.e.*, `NANG1, NANG2, ...`, it is assumed that the first `NANG1` cones will have the same

opening angle and so on. For spheres, if the user omits the number of radii, it is assumed that individual entries will be made (after all, these are user-codes for spherical problems).

```
 NUMBER OF CONES= [NANG(1)[,NANG(2),...,NANG(K)]]
                  # If omitted or ZERO, pure spherical geometry assumed
 NUMBER OF SPHERES= [NRAD(1)[,NRAD(2),...NRAD(J)]]
                  # no needed for individual input
```

Once the user has defined the number of spheres and cones in the problem, the actual values for the radii and angles must be entered, using the keywords outlined below:

```
RADII= RAD(1), RAD(2), ...RAD(j)
                  #radii of spheres defining the geometry
                  #For group input there must be as many entries
                  #as for the NUMBER OF SPHERES, i.e. :
                  #         J = j
                  #For individual input, NRAD(1) must be equal
                  #to the number of entries, i.e.:
                  #        NRAD(1) = j
                  #unless NUMBER OF SPHERES is omitted, in which case
                  #indiviual input is automatically assumed.
ANGLES= ANG(1), ANG(2),...,ANG(3)
                  #The same rules apply for angles as for radii apply.
```

One can also enter a group of regions to be considered as the cavity of a spherical ion chamber and the total dose in these regions will be computed. For CAVSPHnrc, quantities such as $K_{att}$ and $K_{scat}$ and $K_{wall}$ are also calculated for the whole cavity. The specification for the cavity inputs is:

```
CAVITY ZONES= [REG1[, REG2...,REGn]] #geometrical zones defined as the
                                     #cavity (real numbers)
```

### 7.2.2 Material input.

These codes have a simple structure for entering the material input. First the user must provide a list of media in the problem where the first medium is taken as default, *i.e.*, every region is considered to have this medium. Then, medium numbers for all regions where the medium is not medium 1 must be specified.

```
 MEDIA= MEDIUM1, MEDIUM2,..., MEDIUMn

 MEDNUM=         MEDIUM2, MEDIUM2, MEDIUM3,..., MEDIUMn
 START REGION=  START1,  START2,  START3,...,  STARTn
 STOP REGION=   STOP1 ,  STOP2,   STOP3, ...,  STOPn
```

## 7.3 CAVSPHnrc

The NRC user code CAVSPHnrc (spherical geometry) like CAVRZnrc (cylindrical geometry) calculates various factors of interest when using ion chambers such as $K_{att}$, $K_{scat}$, $K_{wall}$ and the dose to the cavity region per unit incident fluence.

The input file for this user code is very similar to the one for CAVRZnrc. Only two input blocks are different, the geometry input block and the input block for the sources. The geometry input was described previously and the input for the sources differ from CAVRZnrc, in that only four source types are available: a parallel beam from any angle (source 0), a point source from any angle (source 1), a parallel beam from any angle with radial distribution (source 10), a point source from any angle with radial distribution (source 11). and a point source from any angle. The source input block is defined by the delimeters `:start source inputs:` and `:stop source inputs:` and the same inputs are needed as in CAVRZnrc (see section 2.7 on page 24). In particular, one must define:

```
 INCIDENT PARTICLE= electron   (-1)  electrons
                    photon     (0)   photons
                    positron   (1)   positrons

 SOURCE NUMBER                 (I)   number of the source
                                     [ISOURC]
 SOURCE OPTIONS                (M)   four or five real numbers as specified
                                     below
```

---

```
 SOURCE 0/10:  FOR PARALLEL BEAM FROM ANY ANGLE (10-->WITH RAD. DISTN)
              RBEAM,UINC,VINC,WINC
               RBEAM   RADIUS OF THE BEAM AT THE FRONT OF THE TARGET IN CM
                               DEFAULTS TO MAX RADIUS
               UINC    INCIDENT X-AXIS DIRECTION COSINE
               VINC    INCIDENT Y-AXIS DIRECTION COSINE
               WINC    INCIDENT Z-AXIS DIRECTION COSINE
                       NOTE: (UINC,VINC,WINC) GET AUTOMATICALLY NORMALIZED
                             DEFAULTS TO (0.0,0.0,1.0)
```

---

```
 SOURCE 1/11:  FOR POINT SOURCE INCIDENT FROM ANY ANGLE (11-->WITH RAD. DISTN)
              DISTR,RBEAM,UINC,VINC,WINC
               DISTR   DISTANCE OF THE SOURCE FROM THE MIDDLE OF THE TARGET
                       IN CM (DEFAULTS TO 100.)
               RBEAM   RADIUS OF THE BEAM AT THE FRONT OF THE TARGET IN CM
                               DEFAULTS TO MAX RADIUS
               UINC    INCIDENT X-AXIS DIRECTION COSINE
               VINC    INCIDENT Y-AXIS DIRECTION COSINE
               WINC    INCIDENT Z-AXIS DIRECTION COSINE
                       NOTE: (UINC,VINC,WINC) GET AUTOMATICALLY NORMALIZED
```

```
                              DEFAULTS TO (0.0,0.0,1.0)
-------------------------------------------------------------------------------

 SOURCE 10 OR 11:
       SPECIFY MODE:
               MODE = local (0)     IF RADIAL DISTRIBUTION IS TO BE INPUT
                                    LOCALLY WHETHER THROUGH THE KEYBOARD
                                    (INTERACTIVE USE) OR THROUGH THE
                                    .INP FILE (DEFAULT)
                    = external (1)  IF THE DISTRIBUTION IS TO BE INPUT
                                    VIA AN EXTERNAL FILE
       IF MODE=local SPECIFY:

           RDISTF(I)= TOP OF RADIAL BIN I FOR I=1,NBIN
           RPDF(I)= PROBABILITY OF INITIAL PARTICLE BEING IN BIN I FOR
                    I=1,NBIN.

                      PROBABILITIES DO NOT NEED TO BE NORMALIZED
                      BUT SHOULD BE IN UNITS CM**-2

       IF MODE=external SPECIFY:

           RDIST FILNAME = FILENAME(WITH EXT) CONTAINING THE ABOVE INFORMATION


       SPECIFY:
           DISTRIBUTION DATA = NONE => NO DISTRIBUTION DATA IN OUTPUT SUMMARY
                             = OUTPUT SUMMARY => INCLUDE DISTRIBUTION
                               DATA IN OUTPUT SUMMARY
```

## 7.4 EDKnrc

The NRC user code EDKnrc can be used to calculate Energy Deposition Kernels for photons or electrons (monoenergetic or polyenergtic) forced to interact at the centre of a spherical geometry[38]. The code can output energy deposition kernels (EDK), dose distributions in the phantom or the dose to regions defined as the cavity of a spherical ion chamber. Voxels are defined by the intersection of a spherical shell with two cones. See figure 3 for more details.

Although the geometry inputs for this user code are similar to CAVSPHnrc, there are some major differences in other inputs. The input block for I/O control, defined by the delimeters `:start I/O control:` and `:stop I/O control:`, is severely abbreviated. It includes an entry, `PRINT OUT EDK FILE` that defines whether energy deposition kernels will be output in the same format as the ones calculated by Mackie *et al.*[37]. The entire input for this block is shown below:

```
:start I/O control:
```

```
  IRESTART
       = first    (0) First run for this data set
       = restart  (1) Restart a previous run
       = analyze  (3) Just read in the raw data and do the statistical analysis
       = parallel (5) Combine results from previous parallel runs
  STORE DATA ARRAYS
       = yes             (0) Store data arrays for re-use
       = no              (1) don't store them
  PRINT OUT EDK FILE
       = yes             (0) EDK stored in old format files
       = no              (1) don't produce EDK files in old format
:stop I/O control:
```

The input block defining Monte Carlo parameters (delimited by `start/stop Monte Carlo inputs:`) is also abbreviated. Here one specifies only the number of histories, the initial random number seeds, and a variable `IFULL`, which specifies the type of calculation, and an input specifying whether doppler broadening is to be taken into account during Compton interactions.

```
IFULL= cavity calculation        #(0) calculate dose in cavity regions
     = energy deposition kernels #(1) calculate and output EDK's
     = dose calculation          #(2) calculate and output dose
     = dose and edk              #(3) calculate and output EDK's and dose

DOPPLER BROADENING= On
                  = Off
```

EDKnrc allows for only three possible sources: 1) a photon source algorithm that forces photons moving along the Z-axis to interact at the origin (source 0) 2) an isotropic point source at the origin for any type of particle (source 1) 3) same as source 0 but with interaction point shifted to a user-specified position on the Z-axis (source 2). Source 2 was left for comparison with older EDK calculations, but the user is strongly discouraged from using it, since it has been shown to produce numerical artifacts when computing EDK's. For accurate EDK calculations source 0 should be used. The inputs specifying the source type, which is included within the `start/stop Source Inputs:` delimiters, are shown below:

```
SOURCE NUMBER= 0 | 1 | 2
#     0 ==>  Photon moving along Z axis forced to interact at origin
#     1 ==>  Point source at origin, isotropically radiating into 4 Pi
#     2 ==>  Same as 0 but interaction point as in old code

# if SOURCE NUMBER= 2
    ZIN      #-> source offset on Z-axis
             #   Option used to emulate old way of calculating EDK
```

Note that in the case of source 0 or source 2, the `INCIDENT PARTICLE=` (standard for all user codes when specifying the source) input must be set to `PHOTON`.

The energy deposited in the geometry can be separated into different contributions from each photon scattering order (*eg.* primary, first scatter, second scatter, multiple scatter and radiative). For electrons, the deposited energy can be split into primary and radiative contributions. In the standard output file `*.egslst`, only the total and primary components are written. ONLY if the user selects the option for creating old format EDK files, all components are stored to a file following the convention:

- `edk[EIN].keV`, for monoenergetic sources, where EIN is the initial energy in keV.
- `file_name.keV`, for polyenergetic sources (spectrum), where `file_name` is the standard output file name

The user also has the choice to create xmgrace plot files for the **total dose** by using the input block for plot control delimited by `:start plot control:` and `:stop plot control:`. A description of this input block is given below:

```
:start plot control:

PLOTTING
       = Off          (0)   no plots or plot files to be prepared
       = Histogram    (1)   histogram plotting
       = Point        (2)   xy graph


ONLY IF not PLOTTING= Off

PLOT RADIAL REGION IX  (M)  radial regions to plot vs angle
                            (= 0 for no plots)

PLOT CONICAL REGION IC  (M)  angular intervals to plot vs radius
                            (= 0 for no plots)

:stop plot control:
```

Plots in radial regions are written to the file `inputfile.angplot` (*i.e.* dose versus angle) and plots in conical regions are written to the file `inputfile.radplot`.

The output capabilities of this user code are very limited but can be easily extended to print out all components of the energy deposition kernels.

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