Action to facilitate the use of Monte Carlo simulation software

The use of Monte Carlo simulation in Gamma spectrometry is getting more and more interest since it can be run on PCs. Such approach is useful for different kinds of calculation, such as:

- Efficiency calibration
- Efficiency transfer
- Coincidence summing corrections

There are two kinds of software which can be used for these:

- Dedicated: GESPECOR, DETEFF, etc.
- Generalist: PENELOPE, GEANT, MCNP, etc.

The dedicated codes are conceived with an user-friendly interface and can be directly applied to derive the calculation results from input data.

On the contrary, the use of generalist codes need some training in order to derive the information of interest. One of the typical difficulties is the preparation of the input files which allows to describe the geometrical conditions, since these must be written with a specific format.

To facilitate the use of generalist Monte Carlo (MC) simulation software, it is proposed to prepare geometrical files for a selection of detectors (HPGe) and measurement conditions. This should include volumic samples and external shielding. It is planned to provide examples to test the use of the MC codes with the prepared geometries, to calculate practical values, such as total or full-energy peak efficiency or coincidence summing corrections for selected radionuclides. Finally, this practical material should be available on the ICRM GSWG web page, so that new users may train themselves.

This ICRM GSWG proposed action could held according to the following steps:

1. Interest of participants: what kind of detectors and samples geometries, MC codes, etc. Different sub-groups of participants could be defined according the MC code they use.

2. Prepare benchmark files for the different Monte Carlo software by the different groups.

3. Use MC codes with these models to compute:

   - Full-energy peak and total efficiencies for point source

   - Coincidence summing for some typical radionuclides

4. Provide the material (input files and calculation results) on the ICRM GSWG web page.

5. Repeat steps 2 to 4 for different geometries

Step 1 : Interest of participants

We received feedback from participants using 4 generalist codes (EGS, GEANT, MCNP and PENELOPE) and 2 dedicated software (DETEFF and GESPECOR).

Step 2: Benchmark files

The participants are contributing to prepare benchmark files specific to the different MC codes. Two cases must be considered since GEANT code, which is object-oriented and run under UNIX, must be compiled including the geometry while the other codes are written in FORTRAN and run with an external geometry file.

To test the feasibility of the action, it is suggested to start with the simple models which were defined by Tim Vidmar in the exercise he led a few years ago, with simple cylindrical detectors (See Annex 1). Some of the participants have already these geometry files and it could be easy to prepare a first set of input data for these simple cases and come to an agreement between the participants on a common structure.

There will be 8 files (2 detectors X 4 sources): I propose to use the following "names" to identify the different geometries:

Name	**Detector**	**Source**
AP	A	Point
AW	A	Water
AS	A	Soil
AF	A	Filter
BP	B	Point
BW	B	Water
BS	B	Soil
BF	B	Filter

It will be necessary to define a file structure that could be easily modified by an external user or by a dedicated user-friendly code. (This is already available for GEANT and further in the course of this action, it is planned to prepare such a facilitating tool with a visual interface to input the geometrical dimensions from generalist pre-defined shapes).

The exchanges between participants should result on the 8 input files for the different codes.

Step 3: Numerical examples

Use MC codes with these models to compute:

- Full-energy peak and total efficiencies for point and volume sources for selected energies

This part of the action could start on early 2018, or, even earlier if input geometries have been agreed among the participants.

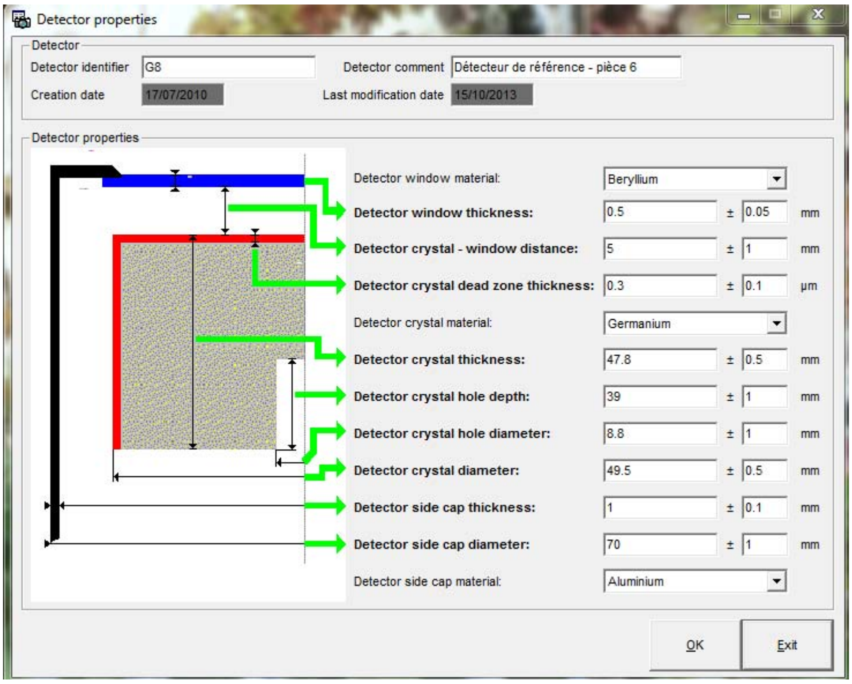
Step 4: Comparison of the first results

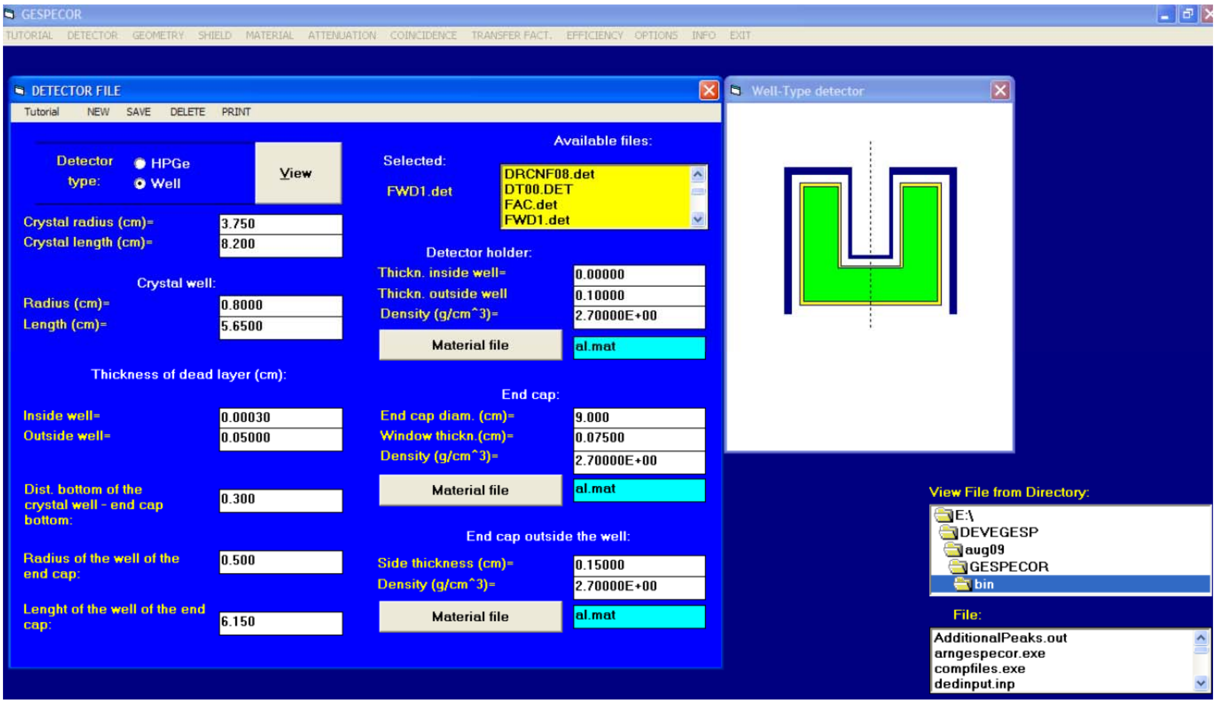
Agreement on validated basic models

Possibility to change the dimensions via an external interface

This will be discussed during the ICRM GSWG meeting that will be held on June 14, 2018.

Examples of interface for input of detection geometrical parameters (ETNA and GESPECOR code)





Annex 1: (from Tim Vidmar)

Equivalence of computer codes for calculation of coincidence summing correction factors

Instructions for participants

A set of well-defined detector and sample geometries is considered. In all the cases, a complete cylindrical symmetry of the sample-detector geometry is assumed. The parameters of the two simulated closed-end coaxial HPGe detectors, a p-type and an n-type one, are given in Table 1, and a sketch of the p-type detector in combination with a point source is also provided (Figure 1). The two detectors are identical, except for the thickness of their respective dead layers. No source containers are to be simulated in this step. In the calculations, the sources should all be placed at a distance of 1 mm from the detector window.

A cylindrical lead shielding should also be included in the simulations. It has both a diametre and a height of 400 mm and its thickness on all sides is 50 mm. The detector is placed centrally within the lead shielding, with the central points of the shielding itself and of the detector crystal coinciding. This leaves a gap of 110 mm between the detector housing and the lead shielding on all sides.

The characteristics of various materials used in the constructions of the detector and sample models are given in Table 3.

Parameter	**Detector A**	**Detector B**
Crystal material	Ge	Ge
Crystal diameter (including the side dead slayer)	60	60
Crystal length (including the top dead layer)	60	60
Dead layer thickness (top and side)	1	0
Hole diameter	10	10
Hole depth	40	40
Window diameter	80	80
Window thickness	1	1
Window material	Al	Al
Crystal-to-window distance	5	5
Housing length	80	80
Housing thickness	1	1
Housing material	Al	Al

Table 1: Detector parameters. All dimensions and given in millimetres (mm). The housing diameter is in all cases the same as the window diameter.

Parameter	Water	Point	Soil	Filter
Sample diameter	90	-	60	80
Sample thickness	40	-	20	3
Sample material	Water	-	Dirt	Cellulose
Sample-to-window distance	1.0	1.0	1.0	1.0

Table 2: Sample parameters. All dimensions and given in millimetres (mm).

Material	Density	Chemical formula
Ge	5.323	Ge
Al	2.70	Al
Water	1.0	H_2O
Dirt	1.4	SiO_2
Cellulose	0.3	$C_6H_{11}O_5$

Table 3: Characteristics of various detector and sample materials. All densities are given in g/cm^3.

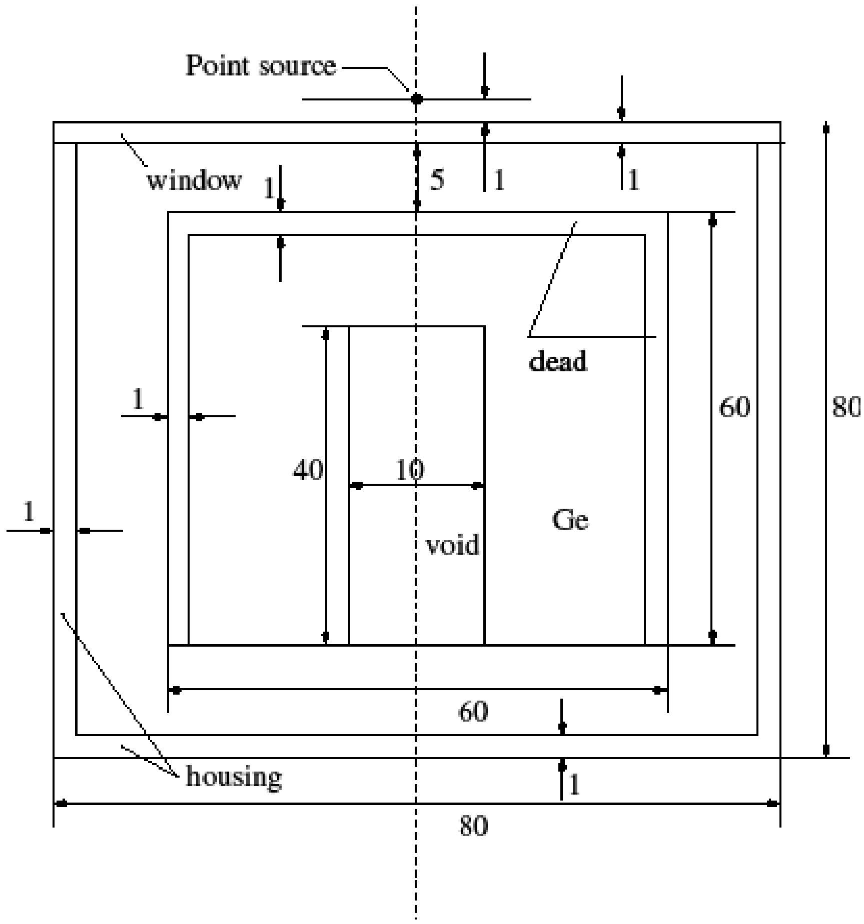


Figure 1: A schematic presentation of the setup for the case of the point source and the p-type detector model.