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THE BASIC CONCEPTS OF GEOMETRY MODELLING AND CAD-INTERFACE IN RTS&T CODE

O.A. Liashenko and I.I. Degtyarev
Institute for High Energy Physics,
Protvino, Russia, 142284
liashol@mail.ru; degtyarev@mx.ihep.su

ABSTRACT

The efficiency of geometry presentation system for investigated objects is one of the most significant factors determining quality of the Monte Carlo programs for radiation transport in heterogeneous 3D-geometries. The most developed of such programs have geometrical modules using a principle of combinatorial geometry, as it was made for the first time in Ref. [1]. The combinatorial geometry module of the RTS&T multi-particle transport code [2] and it applications are described.

Key Words: radiation transport, geometry modelling, visualization

1. RTS&T GEOMETRY MODULE

The RTS&T (Radiation Transport Simulation and Isotopes Transmutation calculation) code [2] includes an effective geometry definition system provided with a combinatorial method. Universal geometry module GEOMETRY [3] basically was intended for the performing of two functions:

- detailed description of the spatial geometry and material composition of considered system
- localization of the site of transported particle in this system.

In the framework of the combinatorial approach the geometry of any physical object can be extremely precisely approximated by set of geometrical regions limited by closed surfaces, filled by homogeneous material and having the constant reflection coefficient. The representation of geometry of a system as combination of geometrical regions is generally ambiguous and it is a problem of combinatorial topology solved in this case by a method of covering of investigated object's space by a system of subsets of Euclidean space.

1.1. Shapes definition

The surface form of each region must correspond to one of the primitives from an available set. More than 30 primitive shapes are defined in the current code version, some of them are shown in Fig. 1.

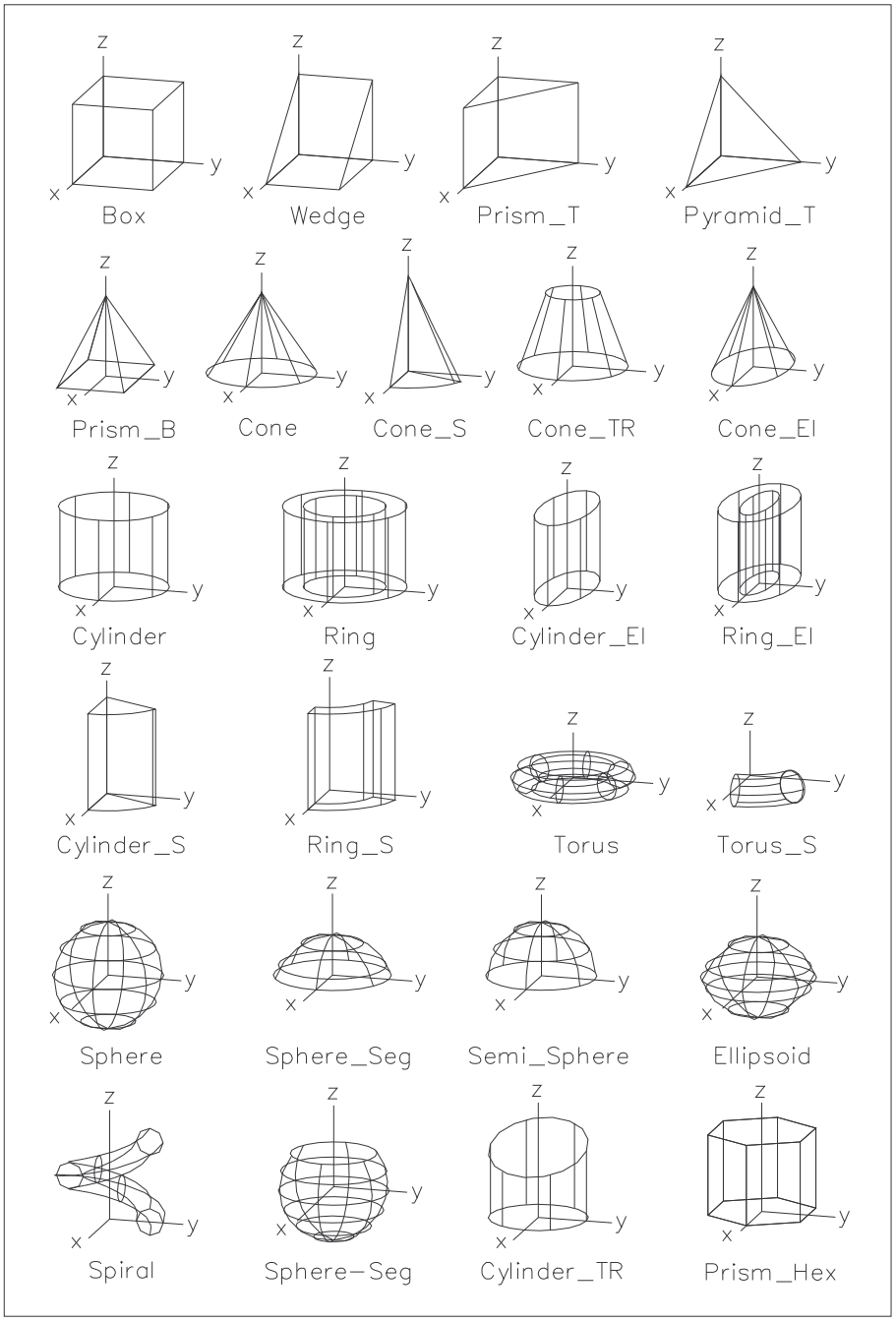

Figure 1. RTS&T set of the shapes.

The recursivial coordinate surface method is used in effective algorithms for analysis whether the considered point is into the region limited by the given surface form. This method allows to define the shape surface by set of equations of the type $u = f(\vec{r})$, where u is one of coordinate variables and $\vec{r} = (x, y, z)$ is a considered point (generally in arbitrary coordinate system). The

falling of the point into any region can be always described by finite number of inequalities [4]. Thus even the definition of very complex primitive shapes isn't a problem. Each shape is characterized by size parameters and has an own local coordinate system.

1.2. Hierarchical embedding tree

The complex 3D geometry can be constructed with Boolean algebra operations (union, intersection, substraction) on the primitive shapes with arbitrary position and rotations. Let the considered system be defined by set of geometrical regions $\{S_n\}$, $n=1, 2,\ldots, N$. The region S_{n1} will be embedded in S_{n2}: $S_{n1} \subset S_{n2}$, if S_{n1} is wholly in S_{n2} and these regions don't coincide:

$$S_{n1} \subset S_{n2} = \vec{r} / \forall \vec{r}:(\vec{r} \in S_{n1} \Rightarrow \vec{r} \in S_{n2}) \wedge (\exists \vec{r}:(\vec{r} \in S_{n2}) \wedge (\vec{r} \notin S_{n1})),$$

where $\vec{r} = (x, y, z)$ is a point in a cartesian coordinate system. We shall name the embedded region S_{n1} the daughter region in relation to the mother region S_{n2}. In addition it is supposed, that the transitivity property is not saved and each region has only one mother: $S_{n1} \subset S_{n2} \subset S_{n3} \Rightarrow S_{n1} \not\subset S_{n3}$. All geometrical regions are numbered in any order by numbers from 1 to N, where N is the total number of regions, and the mother region number of each region is specified in an explicit form. If it is necessary, some regions with a homogeneous material can be united and get a common number. The optimization algorithms for hierarchical embedding tree analysis use the information about a previous particle history.

1.3. Region positioning

The beginning of a local coordinate system serves an origin point. The positioning of the region in the space is defined by position and rotation of local coordinate system in relation a coordinate system of the mother region. Position and rotation of a coordinate system of the most external region are arbitrary in relation to some global coordinate system. The special service routines form geometry input files for often-used configurations (e.g. periodical structures, core cells, mathematical phantoms, etc.) automatically.

1.4. Boundary localization

The GEOMETRY module includes two alternative boundary localization packages based on the different approaches. In the first case the coordinates of the boundary intersection point can be found by iterative way. The second approach requires the alternative definition of each primitive shape by the combination of surfaces bound it (quadric method). The boundary intersection point is calculated analytically as the result of the simultaneous solution of the system of equations describing the surfaces bound the region and the particle trajectory. In case of the very complex shapes it may be difficult to get analytical equations for very complex surfaces, and the number of equations can increase.

If the first method of boundary localization is used, in a general case, when the particle trajectory is simulated using continuous energy loss model and the Moliere theory for angular deflection in a system containing of magnetic field a maximal step-size can be estimated as

$$\Delta t^{\max} = \begin{cases} \min\{\lambda, \Delta t^{geom}, \Delta t^{ion}, \Delta t^{Moliere}, \Delta t^{field}\}, & charged \\ \min\{\lambda, \Delta t^{geom}\}, & neutral \end{cases},$$

where λ is the average free-path length to discrete interaction, Δt^{geom}, Δt^{ion}, $\Delta t^{Moliere}$, Δt^{field} are the partial step limitation conditions, connected with follows requirements:

- total ionization cross section is asymptotically to be a constant
- Moliere approximation of multiple scattering is to be valid
- variation of the magnetic field along a step of trajectory is to be small

$$\Delta t_{cm}^{ion} = \frac{\Delta}{dE/dx}$$

with [8]

$$\Delta = \begin{cases} 0.25, & X_0 < 2\ см \\ 0.25 - 0.2/\sqrt{X_0}, & X_0 \geq 2\ см \end{cases},$$

$$\Delta t_{cm}^{Moliere} = \begin{cases} E^2\beta^4 / \chi_{cc}^2 Z_{part}^2 \ln(b_c E^2 \beta^2 / \chi_{cc}^2), \\ for\ leptons \\ (E^2\beta / 0.0141 \cdot Z_{part})^2 X_0, \\ for\ hadrons\ and\ ions \end{cases}$$

Here, X_0 is the radiation length, and Z_{part}, b_c, χ_{cc}^2 are the particle effective charge and material-depended parameters of the Moliere theory, respectively. Δt_{cm}^{field} can be estimated as [11]:

$$\Delta t_{cm}^{field} = \min\{\delta_1, \delta_2, \delta_3\},$$

$$\begin{cases} \delta_1 \approx \Delta B / 4\sqrt{2}B \\ \delta_2 \approx step^2 / R_0^2 \\ \delta_3 = step \cdot \beta / p \end{cases},$$

where B, ΔB, R_0 and p are a value of the field averaged on the trajectory step, a curvature radius for the particle trajectory on the step, variation of the magnetic field along the step and initial particle momentum, respectively.

Thus, the upper limit for transport step for neutral particles is limited by the characteristic size of a geometrical region or the average free-path length to discrete interaction. In many particular cases (for example, for construction of neutral particles trajectories in extended objects with

small-sized heterogeneities) this approach is extremely inefficient. The analytical boundary localization approach hasn't a geometrical limitation of the transport step. The comparison of efficiency of the analytical approach and the iterative approach is shown on fig. 2. Solid curve present the efficiency ratio as a function of a number of one-level objects, dotted curve shows the efficiency ratio as a function of an embedding levels number.

On the base of the unified input data format the combined algorithm which is taking into account a features of reviewed localization methods has been developed and tested.

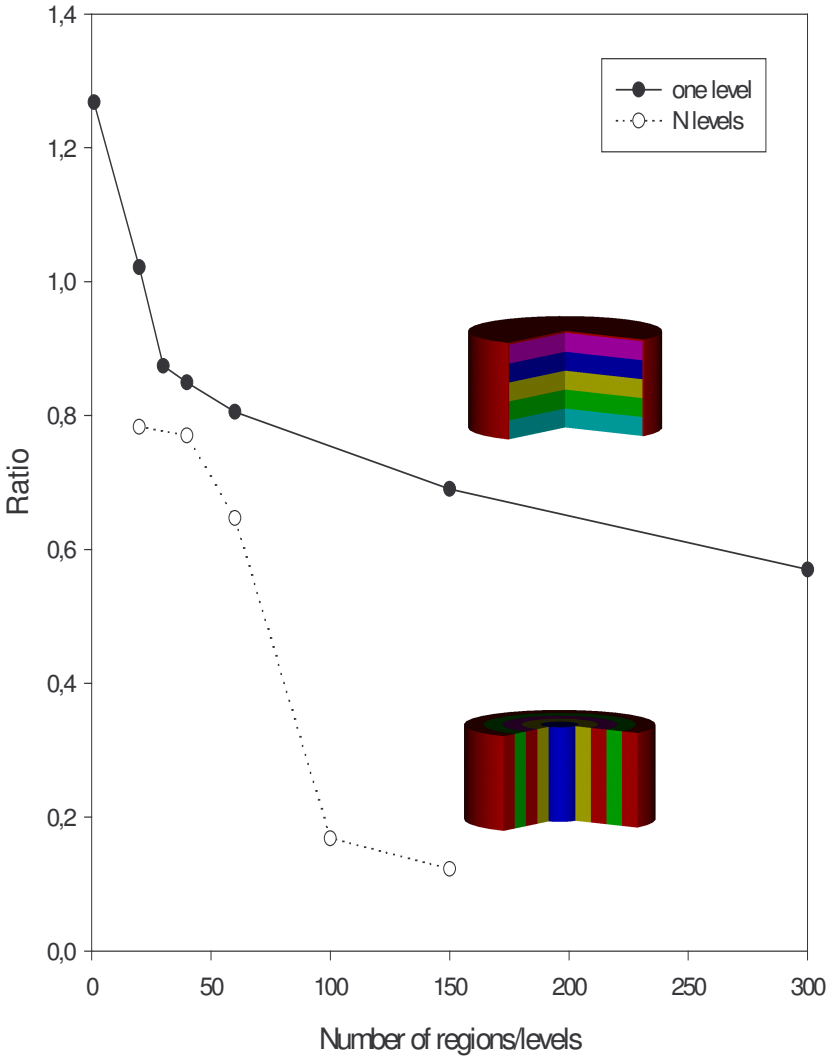

Figure 2. The efficiency ratio for different localization methods.

2. RTS&T-CAD-INTERFACE

The role of graphical supporting tools for geometry verification and output analysis is indisputable. There are two basical approaches to the solution of the problem of visual presentation of investigated object's geometry:

- creating the own graphic application interpreting the geometry input language [5, 7];
- using of a program interface to widely used graphical complexes, predominantly to CAD/CAM/CAE-systems [8, 9].

The most essential advantages of the second approach chosen by us are

1. the great portability and compatibility with other graphical applications and modern hardware for graphical data input (scanner, tomograph, etc.);
2. supporting of the powerful graphical tools of CAD-systems.

4.1. DXF format

The RTS&T geometry input data transform into the format ASCII DXF® (Drawing Interchange Format), designed by the Autodesk company as a standard for exchange by graphic information between AutoCAD® and other applications. DXF format has been chosen for several reasons. This is simple and well documented format. As many modern programs support operation of importing into DXF-format, there are accessible large capabilities of popular CAD-systems which make not only possible the high quality vectorial visualization of three-dimensional objects with zooming, scaling, with an arbitrary rotation in the screen space, with control of layers' properties, with hidden lines removing, etc., but they provide also the preparing of full designer documentation.

4.2. Graphical libraries

The designed program interface allows generate output files in DXF format automatically, without the necessity to know the DXF structure. For this purpose the graphical library of basic CAD-entities (such as text, line, arc, circle, 3D-face etc.) has been designed. The library supports all necessary properties: layer; color; line type etc. and serves as a basis for other library of special routines forming three-dimensional DXF-image of each shape (Fig. 1). The complex geometry visual model is constructed as a composition of simple shapes images at using the tree decoding routine transforming the coordinates of each shape to the global coordinate system.

4.3. Output files

All RTS&T output files in DXF format represent the wire frame visualization of three-dimensional geometry model of considered system but have different intentions.

The first two files provide the facility to display by different colors the material composition or regions arrangement of complex object (Fig. 3) and serve for the need to demonstrate the validity of the geometry models employed. A wire frame representation of the geometry is particularly helpful for checking the component positions in complex hierarchical system. The opening of these files in a graphical application allows to use the mouse pointer to identify the coordinates of any point on the image and to measure the distance between two selected points automatically, to choose to display global coordinates or local coordinates for the complicated objects, to change the user's viewpoint arbitrarily, to apply the zooming to small details or large objects and to use other helpful options for the manipulating by an image and the component placements checking and the editing options for preparing of the drawing suitable for pasting directly into reports.

The third file is used to display particles trajectories in investigated system (Fig. 4). The wire frame geometry image combines with multi-colored particles tracks. The different colors correspond to different particles types. This can be used to better understand how the particle are being transported through geometry and allows to verify initial source location and orientation and to make some conclusions about modeling process.

The other files demonstrate output functional distributions (Fig. 5). The geometrical regions will be drawn by different colors according to the displayed color scale representing the range of values. This facility allows easily interpret large volumes of calculation output. GEOMETRY routine is written in FORTRAN 90 language, according to the ANSI standard.

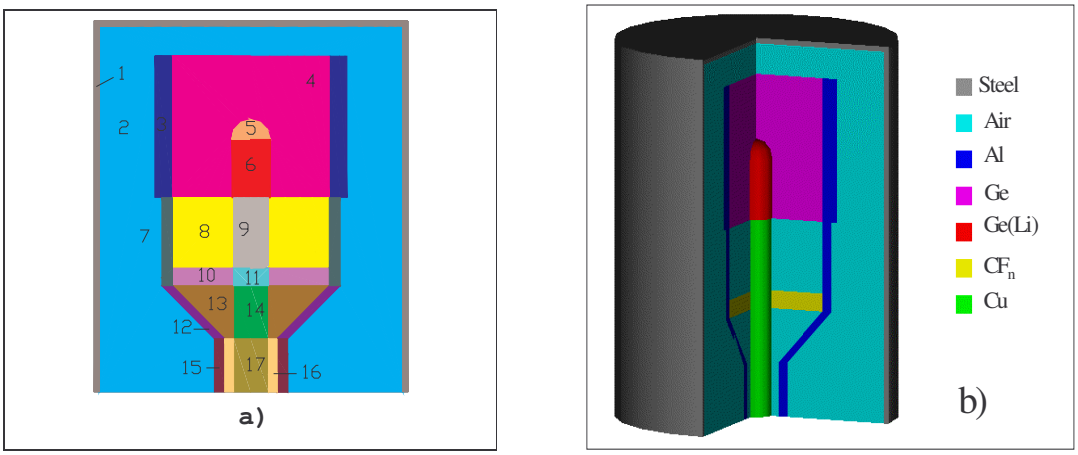

Figure 3. A semiconductor detector geometry example: a) division into regions (frontal projection); b) material composition.

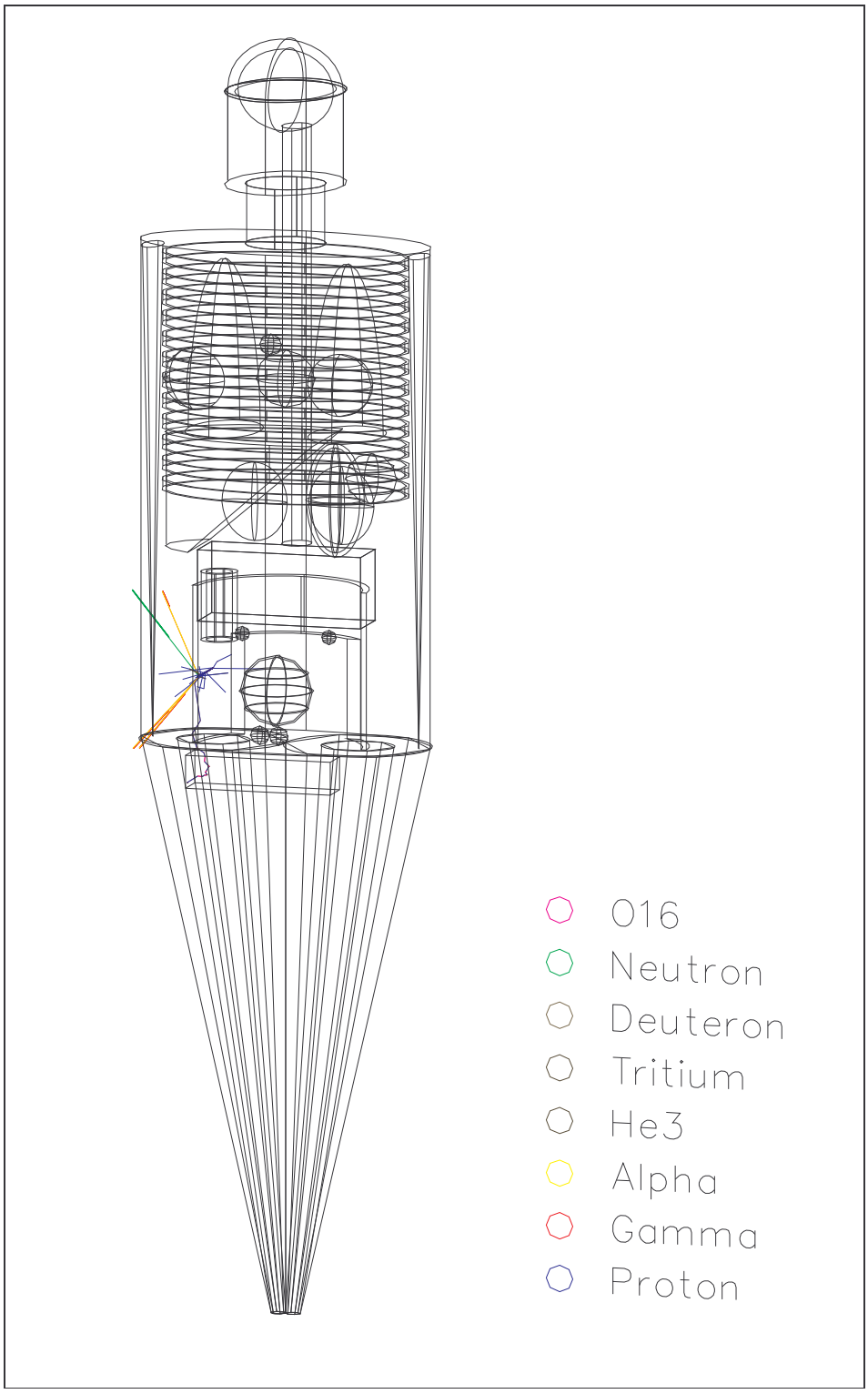

Figure 4. Visualization of particle trajectories in the ORNL mathematical phantom [10].

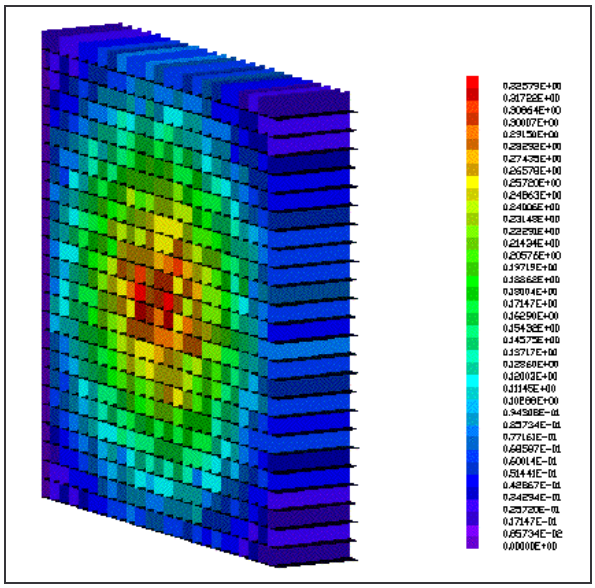

Figure 5. Visualization of output functionals.

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