

A versatile approach for Monte Carlo simulation of tomographic systems

Lucretiu M. Popescu and Robert M. Lewitt

Abstract—In this paper we present the design principles and the main features of a new Monte Carlo simulation code for tomography that, through a modular object oriented approach, maintains the efficiency of specialized solutions while incorporating features common to general Monte Carlo particle transport simulation packages such as the presence of a comprehensive geometrical modeling subsystem. The simulation of photon history through a heterogeneous medium is treated as a distinct case of particle transport, rather than a geometrical representation problem, leading to efficient tracing through voxel-based anthropomorphic phantoms. The approach is general and flexible allowing for a mixed voxel and surface based representation of the attenuation distribution (similarly for the activity distribution). Various variance reduction techniques are introduced.

I. INTRODUCTION

THE Monte Carlo method for particle transport simulation has proven to be a powerful tool in the field of medical imaging. Its various applications, as well as its limitations have been comprehensively presented in recent publications [1], [2].

The Monte Carlo method popularity has lead to the development of various codes, many implementing ingenious techniques that efficiently address specific issues encountered by their authors. The flexibility and extensibility of such codes is often limited by the very presence of such specialized techniques, or by other design options introduced early in their development (restrictions in representing the attenuator medium or the activity distribution, limited detector geometries, etc.). On the other hand the general Monte Carlo simulation packages, like MCNP [3], GEANT [4], [5], or EGS [6] are less frequently employed in diagnostic imaging applications than one would expect given the powerful modeling tools such codes include. Besides long and difficult learning curves one explanation comes from the fact that the generality is often achieved with some loss in efficiency.

In this paper we present the design principles and the main features of a new Monte Carlo simulation code for tomography that, through a modular object oriented approach, maintains the efficiency of specialized solutions while incorporating features common to general packages such as the presence of a comprehensive geometrical modeling subsystem.

II. ARCHITECTURE OF THE SIMULATION APPROACH

In Fig. 1 are schematically identified the components necessary to be modeled in an emission tomography simulator.

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The authors are with University of Pennsylvania, Department of Radiology, Medical Image Processing Group, 423 Guardian Drive, 4-th floor Blockley Hall, Philadelphia, PA 19104-6021, e-mail: {popescu,robert}@mipg.upenn.edu

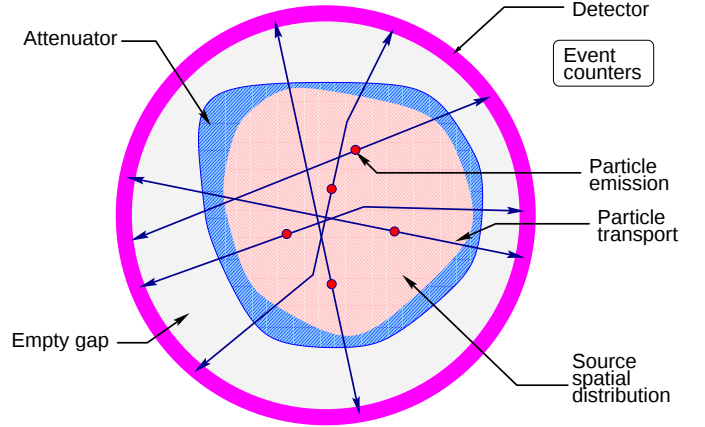


Fig. 1. Diagram outlining the main modules of the simulator

Although the diagram shows the case of a PET scanner, the components represented are the common denominator for most tomography devices using ionizing radiation sources.

From one perspective we can identify components that have a certain physical description (i.e. geometric shape, substance content, position in space): these are the *detector*, the *attenuator*, and the *source spatial distribution* or activity distribution. On the other hand we have the functional components required for the simulation of particle histories. Here we distinguish between the *particle emission* and the *particle transport*. A last class of components are represented by the *event counters*, some of which have physical counterparts in the detection and data acquisition electronics.

A versatile design approach is needed given the variety of possible scanner configurations, the wide range of shapes and form of representation for the attenuator and source spatial distribution, and the multitude of specific tasks to accomplish through simulations in an optimal manner. Each of the above components must be able to instantiate specific versions while preserving a uniform interface with the rest of the system (see in Fig. 2 the modules and their functional dependencies). A natural candidate for achieving this goal is the use of inheritance and polymorphism features offered by the object oriented programming languages. We have used C++, and the above generic modules with all derived versions are implemented as C++ classes.

More details about the function and implementation of each above module are given in the following subsections.

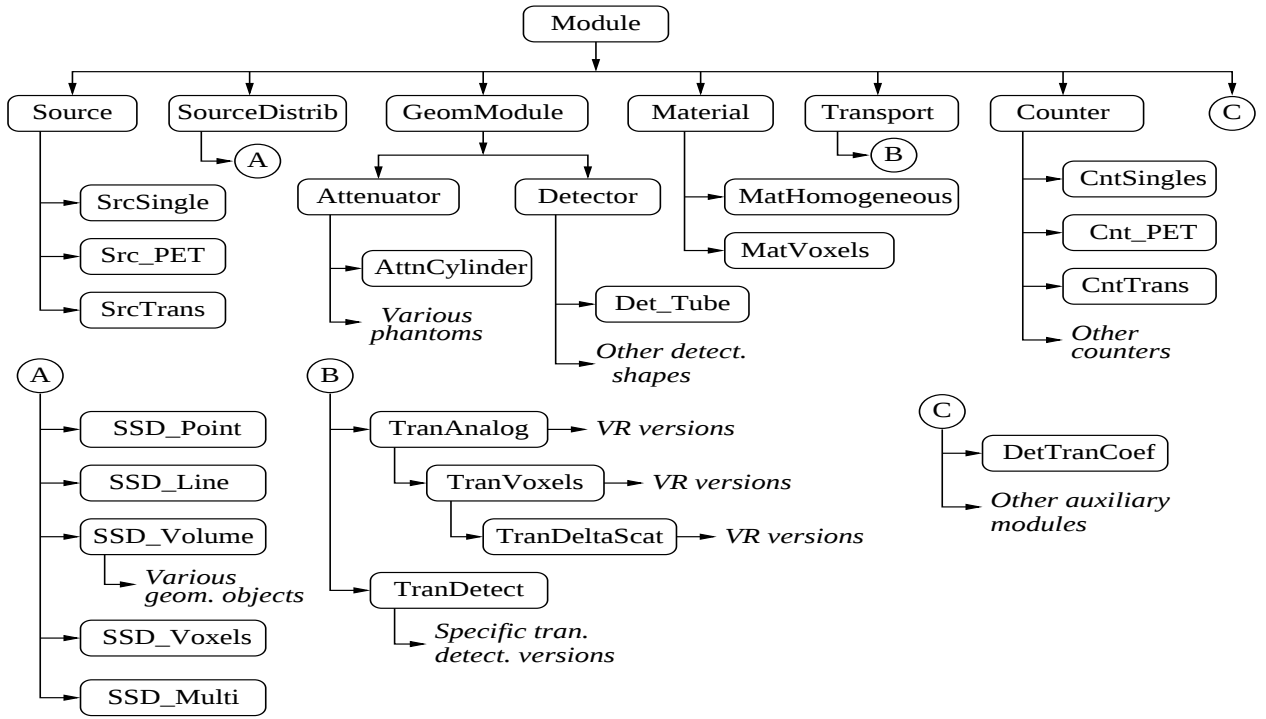


Fig. 3. Class hierarchy. The *Module* class from which are derived all other classes implements the common mechanisms of input and output as well as a multi-step initialization procedure (*à la* Unix System V) providing a uniform and flexible interface with the user. In addition to the main modules described in the text *Source*, *SourceDistrib*, *Attenuator*, *Detector*, *Transport* and *Counter* here is shown the *Material* module which provides the material specifications used by the *Transport* modules. Another category of modules (branch C) consists of the *Auxiliary* modules that perform various tasks that are useful, but not directly required by the simulation, such as deterministic computation of the transmission data, or converting analytically (surface based) defined phantoms into voxelized images. For the sake of clarity the class names shown here have been slightly changed from those in the original C++ code and a series of other simplifications have been made.

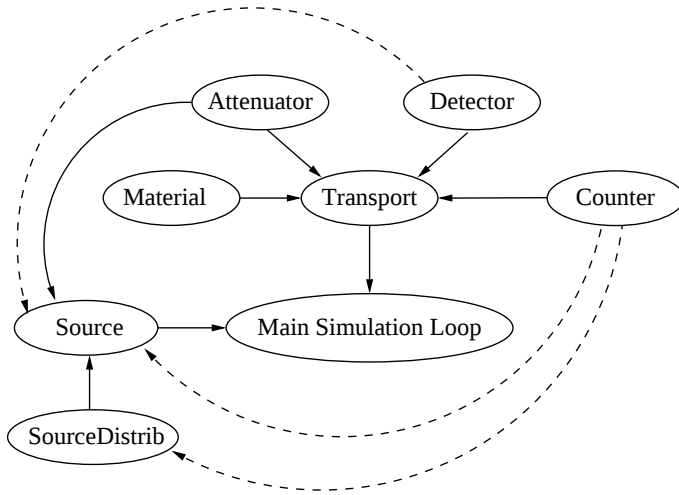


Fig. 2. Module functional dependencies. The dashed lines represents dependencies required when certain variance reduction techniques are applied.

A. Geometrical modules

A Monte Carlo simulation of particle transport is largely a problem of geometry representation and ray tracing. Therefore it would be helpful to have a flexible system for describing the geometry and automatically performing the task of tracing

particles across regions. For photon transport at energies commonly used in nuclear medicine, the effort spent for simulating the interactions is exceeded by the effort spent performing other tasks, most important of them involving the geometry. Therefore the flexibility and generality of the geometry modeling system should be achieved with a minimum overhead cost.

The geometrical aspects of the *detector* and the *attenuator* are represented using such a geometry representation system described in more detail in [7]. Here we will mention only its main features: (1) uses a surface (or boundary) representation technique, thus offering high flexibility in defining various geometrical bodies; (2) provides a mechanism for automatically linking the adjacent volumes; (3) implements a robust tracing method that employs in a systematic manner geometrical reasoning in order to avoid ambiguities induced by floating point rounding errors.

For flexibility the detector and attenuator are represented as distinct entities, while the overall unified geometrical setup is achieved in the following manner: the detector supplies the attenuator with its inner surface and the list of adjacent volumes to this surface. The attenuator completes its setup with the above data and provides the detector with the list of its volumes adjacent to the detector inner surface. The empty gap shown in Fig. 1 is included as part of the attenuator; if a collimator is present it is considered as part of the detector module, given

its intimate relation with the detector array. For each region of the attenuator and the detector, the substance content and an appropriate transport method must be specified.

The *source spatial distribution* modeling is a matter of sampling a spatial density distribution at the request of the *source* module that simulates particle emissions. In the case of emission tomography we can have activity distributions given as geometrical bodies analytically defined or discretized distributions. The sampling is done using Walker's alias sampling technique [8], [9] (described also in [10]). An alternative consists in cyclically stepping through all volume elements for each one generating a number of particles proportional to its activity. The main drawback of the latter approach is that the sequence of detected events is not random, which is undesirable for certain applications such as studies using list-mode data in random succession. In the case of transmission scans the source spatial distribution is the trajectory relative to the object followed by the scanner source.

B. Functional modules

The *source* module simulates the particle emissions assigning their initial values of energy, direction, etc.. Distinct sources for positron annihilation photon pair emission, single photon emission and transmission scan simulations are implemented.

The *transport* modules perform the simulation of particle histories. The transport classes used here are specializations derived from versions developed and tested in previous work [11]. Distinct transport classes are used for modeling of photon detection processes and these initiate the tallying of the detected emission events. The photon cross sections used are those provided by the code XCOM [12]. The Compton interactions for unpolarized and linearly polarized photons are sampled using a general technique described in [10]. The linearly polarized cross section is required in PET simulations in order to treat accurately the case of photon pairs when each suffers at least one interaction, as pointed out by Bice [13]. However, our tests so far involving configurations commonly used in experiments have revealed little noticeable effect of photon polarization.

The *counter* modules are responsible for tallying of the detected emission events according to source type and level of detail required, which are saved in the desired format.

C. Transport through inhomogeneous materials

The modeling of photon transport through a voxel represented distribution of substance is considered as a particular case of the transport class. That is, for one or more regions, usually specified using the geometrical representation system, instead of specifying their content as a homogeneous substance, one can specify inhomogeneous distributions and the appropriate transport method to deal with that distribution. One example is the use of a ray tracing technique in which all voxels along the trajectory are visited individually. A second approach, more general as it is not limited only to the case of voxels, is offered by the method of fictional interactions (or delta scattering) [14] in which for a given space region the interaction positions are sampled using the maximum attenuation coefficient for that

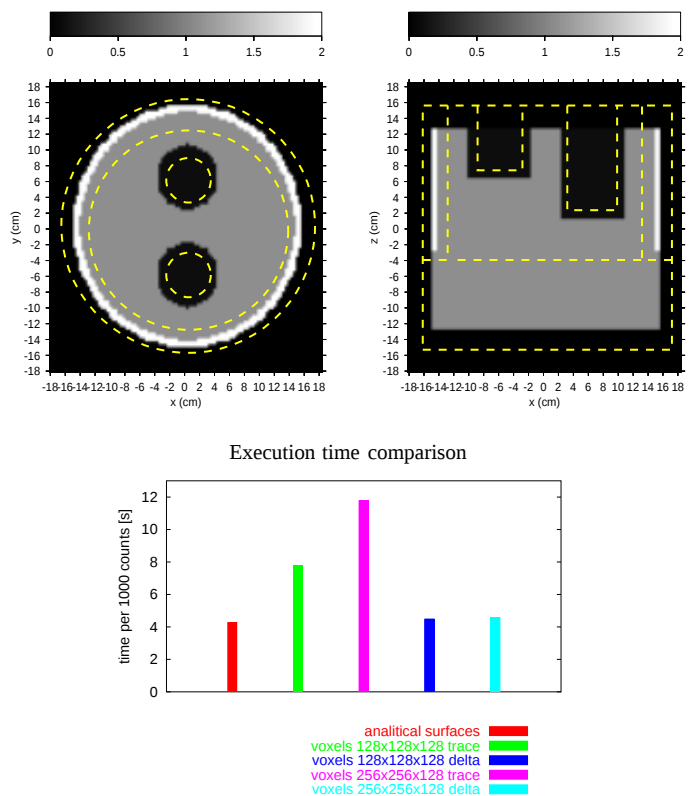


Fig. 4. Example of partitioning of a voxelized Utah phantom in low, medium and high attenuation regions for efficient use of delta scattering method. The execution time is independent of the image resolution and is comparable with that needed for tracing through analytical surfaces only. Time measurements were carried out for a PET source distributed inside the phantom and were performed on a Pentium MMX at 266 MHz CPU running Linux.

region, while the difference down to the local value of the attenuation coefficient is assigned to a fictitious null interaction.

D. Incorporation of variance reduction techniques

Variance reduction techniques can be introduced by deriving new versions of the appropriate functional modules. Briefly these are:

- Sampling of the emission direction function of detector acceptance angles.
- For the case of PET sources we have implemented a technique of particle splitting for the second branch photon if the first branch photon has been detected [15], with a distinct splitting factor if scattered.
- Particle splitting if the photon suffers a first scatter. As shown in Fig. 5 this technique dramatically increases the calculation speed for scatter estimates.
- Sampling only of the Compton scatter, with modification of the photon weight accordingly.
- Restricted Compton interaction that samples photons with energies above a user defined threshold.
- Forced escape from the attenuator (or colimator), coupled with the following technique is often called forced detection [16], [17].
- Forced interaction in detector.

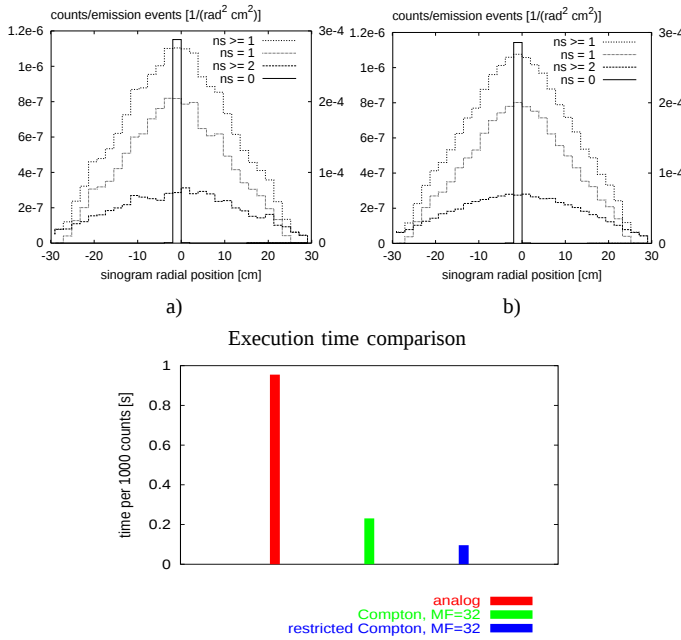


Fig. 5. PET scatter distribution simulation for a point source in the center of a 20×20 cm water cylinder. a) analog simulation; b) simulation using Klein Nishina cross section restricted at 300 KeV and particle splitting for the first scatter event with multiplication factor MF=32. (Time measurements were performed on a Sun SPARC at 500 MHz CPU, running Solaris.)

III. CONCLUSION AND FUTURE DEVELOPMENTS

Through a modular, object oriented approach a new flexible and easy to extend Monte Carlo simulator for emission tomography has been developed. It incorporates a geometry modeling system that facilitates the representation of various detector configurations, collimators and attenuation phantoms. The design option of treating the simulation of photon history through an inhomogeneous medium as an intrinsic transport problem rather than a geometrical representation problem allows for efficient tracing through voxel-based anthropomorphic phantoms, such as Zubal phantom, by confining the high attenuation organs in narrow analytically defined volumes and applying the delta scattering technique. Various variance reduction techniques have been introduced.

The present features implemented so far are motivated by the needs of our current projects, mainly PET system simulations.

The geometry modeling system provides an easily extensible framework and in future work we intend to enlarge the library of detectors in order to adequately treat the case of SPECT or pinhole systems and to adapt other variance reduction techniques more suitable for these applications.

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