Unified Description and Validation of Monte Carlo Simulators in PET

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***Abstract*—Several Monte Carlo simulators are currently available for Positron Emission Tomography (PET). Because each code has been described in a specific way, it is difficult to know which one is best suited to a specific application. To help clarify the specificities and accuracy of different codes, we propose a uniform description of the code features. This description specifies features pertaining to the models used for simulating the physics of PET and describing a PET acquisition, to the acceleration strategies and to the technical characteristics of the code implementation. To assess the code accuracy, we suggest validation procedures based on NEMA phantoms involving standard physical parameters and simulation of a complex activity distribution. A test characterizing the statistical properties of simulated events is also described. The proposed code description and validation procedures are illustrated by considering the SimSET and PET-EGS codes. Despite the numerous differences between these 2 codes as demonstrated by the unified description of the codes, both codes yielded data with properties close to those of real data. Depending on the intended application, one code might be preferred however as the underlying physical models and computer efficiency differ significantly. The proposed code description and validation procedures might help determine which code is best appropriate for a specific application.**

I. Introduction

MONTE Carlo simulations are currently widely used in Positron Emission Tomography (PET) imaging for optimizing detector design and acquisition protocols, and for developing and assessing correction and reconstruction methods [1]. Several Monte Carlo simulators are currently available for PET simulations [1] and new codes are under development [2]. Each code presents some advantages and limits with respect to the others. However, because each code has been described and validated in a specific way, it is difficult to know which code is best suited to a specific application. The purpose of this work is twofold. First, we propose a uniform description of the features of the codes that could help determine a priori whether a code is appropriate for a specific application. Second, we present some validation procedures making use of the NEMA NU2 measurements [3,4] and involving standard criteria (e.g., spatial resolution, scatter fraction, detection sensitivity) that could be performed to characterize the accuracy of a code. Tests appropriate for reporting the computational efficiency of a code are also suggested. The relevance of the proposed code description and validation procedures is illustrated by considering two codes currently available for PET simulation.

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II. Methods

A. Description of a simulator

The current codes available to simulate PET acquisitions can be described by considering four main classes of features: 1) the models used to simulate the physics involved in PET; 2) the models used to simulated a PET acquisition (in terms of activity and attenuation distributions and detector components); 3) the acceleration strategies which determine the efficiency of the code; 4) the technical characteristics of the code which determine its portability and ease of use. The proposed description profile lists precise information related to these four types of features (see Results section). As the aim is to facilitate the comparison between codes, only the features that can differ from one code to another are considered.

B. Validation of a simulator

A relevant use of data generated by a Monte Carlo simulator requires a preliminary validation of the reliability of the data, at least regarding the features that are of interest for the problem to be addressed through simulations. We propose a set of validation tests that could be performed to characterize the accuracy of a code. Because the accuracy of a code is determined by its ability to generate data identical to those that would be acquired on a real imaging system, most tests involve the comparison of simulated and experimental data. For this purpose, the proposed tests use some of the NEMA NU2 1994 and 2001 phantoms [3,4], as this material is widely available. The tests relate to: a) physical parameters characterizing the global response of a PET scanner, b) spatial distributions for homogeneous and heterogeneous radioactive sources, allowing for the assessment of the local response of a PET scanner, and c) statistical properties of the simulated data. All tests are precisely described, in terms of data collection procedure, calculations and analysis, and reporting. Most tests apply to the detected events as sinograms, to avoid any confounding factors that could be introduced by different implementations of tomographic reconstruction. Experimental and simulated sinograms corresponding to each transaxial

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plane (parallel to the detector rings) shall be extracted from the 2D or 3D data using single slice rebinning (SSRB).

Global analysis. The accuracy in simulating the global response of the PET scanner is assessed through 4 parameters.

1) Intrinsic spatial resolution. The intrinsic spatial resolution measurements use part of the NEMA NU2 2001 point source set up. Transaxial spatial resolutions are characterized by the full width at half maximum (FWHM) and full width at tenth maximum (FWTM) of the point spread function for the centered and 10 cm off-centered point source. Axial spatial resolution is reported using the FWHM and FWTM of the point spread function of the centered source.

2) Scatter fraction. The scatter fraction measurements shall be performed according to the NEMA NU2 2001 guidelines. The system scatter fraction corresponding to the average scatter fractions over all slices encompassing the 65 cm central axial FOV shall be reported.

3) System sensitivity. Because the experimental tools required for performing the sensitivity measurements as recommended by the NEMA NU2 2001 procedure are not easily available yet, the sensitivity measurement procedure as described in the NEMA NU2 1994 standard was considered. The total and true axial sensitivity profiles shall be plotted. The total and true system sensitivities shall also be reported.

4) Count rates. The same set up as that used for the sensitivity measurements shall be used. True, randoms and noise-equivalent-count (NEC) rates shall be plotted as a function of activity concentration (kBq/mL) in the phantom.

Local analysis. The reliability of the simulator to model the local response of a PET scanner is assessed by considering the images obtained for homogeneous and heterogeneous radioactive sources.

1) Transaxial activity profile through a homogeneous activity distribution. A transaxial activity profile through the 19 cm long NEMA cylinder used for sensitivity measurements shall be displayed to assess the match between the spatial distribution of the simulated and of the experimental events.

2) Recovery of a heterogeneous-voxelized activity distribution. A specific simulation involving the Zubal [5] numerical phantom shall be performed. Simulated sinograms shall be reconstructed using 2D filtered backprojection (Ramp filter) of the SSRB sinograms. The original activity map shall be displayed together with the reconstructed trues and trues + scatter activity maps. The profiles corresponding to the reconstructed images shall be shown.

Statistical properties of the simulated data. Because some reconstruction procedures assume that the acquired data follow a specific statistical distribution, it is important to verify if simulations preserve the statistical properties of the data, in order to use simulated data to assess reconstruction methods. The same set up as that used for sensitivity measurements shall be used, but 20 equivalent simulations of this set up shall be performed, keeping all parameters unchanged. Similarly, 20 replicated experiments shall be obtained. For each pixel of the rebinned sinogram, the averaged value over the 20 replicates and the associated standard deviation shall be calculated. A plot of the standard deviation values against the averaged value shall be reported, including a number of points equal to the number of pixels in the sinogram.

C. *Computational efficiency of the simulation code*

The computational efficiency of the code can be characterized by the CPU time needed to track a coincidence event and to store the output information. It has to be measured for activity maps analytically described and for voxelized activity maps. Because the simulation time highly depends on the computer system performance, it has to be normalized by a number characterizing the computer performance. We propose to consider a metric provided by the Standard Performance Evaluation Corporation (SPEC) (http://www.spec.org). The same set up as that used for the sensitivity measurement shall be considered for characterizing computational efficiency of an analytically described phantom. For a voxelized source distribution, the set up corresponding to the complex Zubal phantom activity distribution shall be used. For each set up (uniform short cylinder and Zubal phantom), the CPU computing time for the total simulation shall be divided by the number of generated coincidences and by the SPECfp_rate_base2000 (SPECfp_rate_base95 if SPECfp_rate_base2000 is not available from the SPECT Web site). The number of generated coincidences per second normalized to the computer-performance shall be reported.

III. Results

To illustrate the relevance of the suggested description profile and validation procedures, two simulators currently available for PET simulations were considered, namely SimSET [6], and PET-EGS [7]. The original SimSET v2.6.2.3 was slightly modified so that it did not use the depth of interaction information anymore (which is not available using conventional real PET scanners) to determine the line of response. Acceleration strategies were not used in SimSET.

A. *Description of the simulators*

Table 1 summarizes the characteristics of SimSET and PET-EGS following the proposed description profile, according to the description table. References to a more complete description of the simulators are given, when available.

B. *Validation of the simulators*

To illustrate the relevance of the proposed validation procedure, the accuracy of SimSET and PET-EGS was studied by considering experiments performed on the CPET scanner (ADAC/UGM, Philadelphia, PA) and corresponding simulations. The results of the validation procedures are summarized in Table 2 for SimSET and PET-EGS, together with the experimental values measured by CPET.

C. *Computational efficiency of the codes*

Because the SPECfp_rate_base2000 metric was not available for the computers used to run our simulations, we considered the SPECfp_rate_base95 metric. The SimSET simulations were run on a Sun Ultra Sparc 10 workstation, which has a SPECfp_rate_base95 value of 151. The PET-EGS simulations were run on a Sun Enterprise 450 workstation, which had a SPECfp_rate_base95 value of 392 (high SPECfp_rate_base95 value corresponding to high throughput of the machine).

For the short uniform cylinder experiment, PET-EGS generated 93 coincidences /sec, while SimSET generated 1266 coincidences/sec. Normalizing to the computer performance, SimSET was about 35 times faster than PET-EGS for the short uniform cylinder (8.38 coincidence/sec against 0.24). For the voxelized Zubal phantom, PET-EGS generated 162 coincidences/sec, while SimSET generated 2941 coincidences/sec. Taking into account the differences in computer performance, SimSET was about 47 times faster than PET-EGS for the voxelized Zubal phantom (19.48 coincidence /sec against 0.41).

IV. Discussion

The proposed unified description of Monte Carlo simulators aims at facilitating the comparison of codes in terms of features that might affect 1) the code accuracy, 2) the flexibility with which specific configurations can be simulated, 3) the computational efficiency of the code, 4) its practical implementation in a specific environment. All data provided in the description profile should therefore help the user quickly determine whether a code satisfies his need given the intended use of the code. If the description profile corresponding to each PET simulator currently available could be filled in and published, this would probably save a lot of time to people interested in Monte Carlo PET simulation, either to choose the code appropriate for their application, or to know which code offers a specific feature so that they could possibly get hints to add the functionality to another code. Even if there are not that many PET Monte Carlo simulators, going into the details of each simulator is tedious and time consuming. Although the detailed analysis of the features of a code remains definitely necessary at a certain point for properly using and understanding the code, the idea of the unified description profile is to simplify this task by providing a quick but detailed overview of the features of different codes that have been described so far each in a specific way. The original features of codes under development could also be easily identified by referring to the description profile.

It is obviously not possible to give a complete characterization of code features using a one-page summary. Additional information regarding the usefulness of a code can however be provided by illustrating the performance of a code, in terms of how well it reproduces data acquired on a real imaging system. This is the aim of the proposed validation procedures. Again, there is no way one can provide full validation of a code using a one-page summary of the code performance. However, the way key parameters such as spatial resolution, sensitivity, count rates, are reproduced by simulations can still be captured using few figures of merit. Furthermore, using a unified validation procedure would be the only way to compare codes “back-to-back” using the same criteria, similar to the NEMA NU2 standard to characterize PET machine performance.

We applied the proposed description and validation procedures to two PET simulators. Our intend was not to determine which code was the best between the two. Actually, the answer to this question highly depends on the intended use of the code. For instance, PET-EGS should probably be used instead of SimSET in simulation studies focusing on count rate performance of a PET scanner. Because of its greater computational efficiency compared to that of PET-EGS, SimSET seems more appropriate for generating large datasets for evaluation purpose.

V. Conclusion

We introduced a description profile and validation tests for characterizing Monte Carlo PET simulators. The feasibility of a unified description and reporting of the accuracy and computational efficiency of simulators was demonstrated by considering two state of the art Monte Carlo codes: SimSET and PET-EGS. Analysis of other PET simulators using the proposed description and validation procedures could help researchers choose a PET Monte Carlo simulator appropriate for the intended application.

VI. Acknowledgment

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VII. References

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TABLE I

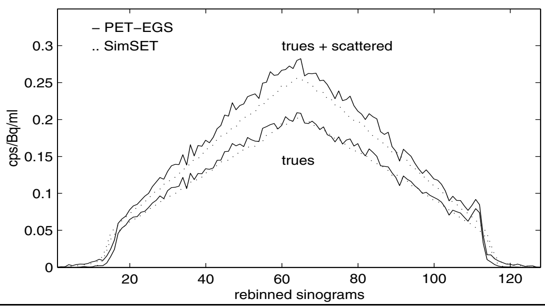
CHARACTERIZATION OF SIMSET AND PET-EGS USING THE PROPOSED DESCRIPTION PROFILE

	SimSET	PET-EGS
Modeling the physics		
Random number generator	Function:Random Periodicity: 16(2e31-1)	Function:Rndm2 Periodicity: 4.6.10e18 (CERN library entry V107)
Photoelectric effect	☐No ☒Yes: EPDL94 (EPDL94)	☐No ☒Yes: PHOTX (Sakamoto, Third EGS4 Users's meeting 1993)
Compton scatter	☐No ☒Yes: EPDL94 (EPDL94)	☐No ☒Yes: PHOTX (Sakamoto, Third EGS4 Users's meeting 1993)
Rayleigh scatter	☐No ☒Yes: EPDL94 (EPDL94)	☐No ☒Yes: PHOTX (Sakamoto, Third EGS4 Users's meeting 1993)
X-rays	☒No ☐Yes:	☒No ☐Yes:
Radioisotope model	☐Full-decay ☒Positron emitter ☐2 511keV gamma emitter	☐Full-decay ☐Positron emitter ☒2 511keV gamma emitter
Positron mean-free path	☐No ☒Yes: ☐*Analytical* ☒*Monte Carlo*	☐No ☐Yes: ☒*Analytical* ☐*Monte Carlo*
Positron uncolinearity	☐No ☒Yes: ☐*Analytical* ☒*Monte Carlo*	☐No ☐Yes: ☒*Analytical* ☐*Monte Carlo*
Photon transport in crystal	☐No ☒Yes: ☐*Analytical* ☒*Monte Carlo*	☐No ☒Yes: ☐*Analytical* ☒*Monte Carlo*
Scintillation photons	☒No ☐Yes: ☐*Analytical* ☐*Monte Carlo*	☐No ☒Yes: ☒*Analytical* ☐*Monte Carlo*
Detector dead time	☒No ☐Yes: ☐*Analytical* ☐*Monte Carlo*	☐No ☒Yes: ☒*Analytical* ☐*Monte Carlo*
Pile-up model	☒No ☐Yes:	☒No ☐Yes:
Backcompartment model	☐No ☒Yes: juxtaposition of empirical layers	☐No ☒Yes: analytical model (Castiglioni et al, IEEE Trans Nucl Sci, 2002)
Random events model	☒No ☐Yes:	☐No ☒Yes: Monte Carlo model (Castiglioni et al, IEEE Trans Nucl Sci, 2002)
Modeling a PET acquisition		
Activity distribution	☒Analytical ☒Segmented voxel-based: 256 levels	☒Analytical ☒Segmented voxel-based: 32768 levels
	☐Unsegmented voxel-based ☒Analytical and voxel-based	☒Unsegmented voxel-based ☐Analytical and voxel-based
Attenuation distribution	☒Analytical ☒Segmented voxel-based: 256 levels	☒Analytical ☒Segmented voxel-based: 32768 levels
	☐Unsegmented voxel-based ☒Analytical and voxel-based	☒Unsegmented voxel-based ☐Analytical and voxel-based
Dynamic distributions	☒No ☐Yes:	☒No ☐Yes:
Transmission acquisitions	☒No ☐Yes:	☒No ☐Yes:
2D acquisition mode	☒No ☐Yes: ☐*HR* ☐*HS*	☒No ☐Yes: ☐*HR* ☐*HS*
3D acquisition mode	☐No ☒Yes: ☒*Fully* ☐*Spanning* ☒*Re-binning* ☐ *HR, HS*	☐No ☒Yes: ☒*Fully* ☒*Spanning* ☒*Re-binning* ☒ *HR, HS*
Interplane septa	☒No ☐Yes: ☐*Analytical* ☐*Monte Carlo*	☒No ☐Yes: ☐*Analytical* ☐*Monte Carlo*
External shielding	☐No ☒Yes: ☒*Analytical* ☐*Monte Carlo*	☐No ☒Yes: ☐*Analytica* ☒*Monte Carlo*
Detector medium	☒Scintillator ☐Solid state	☒Scintillator ☒Solid state
Detector unit	☒Large detector ☐Small detector ☐*Block* ☐*Pixellated*	☒Large detector ☒Small detector ☒*Block* ☒*Pixellated*
Scanner shape	☐Polygonal ☒Ring	☒Polygonal ☒Ring
Scanner motion	☒No ☐Yes: ☐*Rotating* ☐*Translating* ☐*Wobbling*	☒No ☐Yes: ☐*Rotating* ☐*Translating* ☐*Wobbling*
Acceleration strategies		
Geometric approximations	☐No ☒Yes: Acceptance angle	☒No ☐Yes:
Variance reduction techniques	☐No ☒Yes: ☒*Forced detection* ☒*Stratification*	☒No ☐Yes: ☐*Forced detection* ☐*Stratification*
Parallelisation facilities	☐No ☒Yes: ☐*Parallel language* ☒*Parallel runs*	☐No ☒Yes: ☐*Parallel language* ☒*Parallel runs*
Technical characteristics		
Language	C	Fortran, C, matlab
Platforms/operating systems	All platforms operating UNIX	UNIX for SUN platforms
Memory requirements	500 Mbytes	400 Mbytes
User interface	☒*Text* ☐*Graphics*	☒*Text* ☐*Graphics*
Output information	☒Energy ☐Time ☒Spatial coordinates	☒Energy ☒Time ☒Spatial coordinates
	☐Singles ☒Coincident events	☒Singles ☒Coincident events
	☒Trues ☒Scatter:9th order ☐Randoms ☐Multiples: order	☒Trues ☒Scatter:inf order ☒Randoms ☐Multiples: order
Output data	☒Sinograms ☒List ☐Images ☒Energy spectra	☒Sinograms ☒List ☐Images ☒Energy spectra
Output file format	☒Binary ☐Ascii ☐DICOM ☐Constructor	☒Binary ☐Ascii ☐DICOM ☐Constructor
Code availability	☐No ☒Yes: ☒*Public domain* ☐*From authors*	☐No ☒Yes: ☐*Public domain* ☒*From authors*
Technical documentation	☐No ☒Yes	☐No ☒Yes:
Technical support	☐No ☒Yes	☒No ☐Yes:
User group	☒No ☐Yes	☒No ☐Yes:
Test data	☒No ☐Yes:	☐No ☒Yes: www.mi.inb.cnr.it/mcet

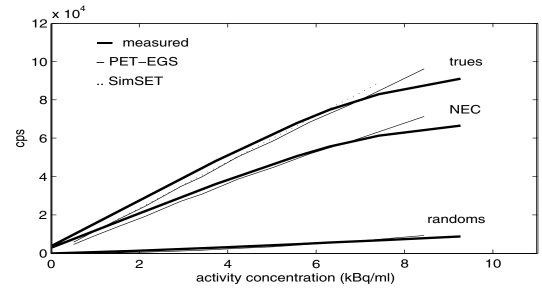
TABLE 2
RESULTS OF THE VALIDATION PROCEDURES FOR SIMSET AND PET-EGS

	Experimental	SimSET	PET-EGS
Transaxial resolution:			
- FWHM/FWTM @ x=0 cm, y= 1 cm	4.8/10.4 mm	5.7/11.5 mm	4.3/9.5 mm
- FWHM/FWTM @ x=0 cm, y=10 cm	6.5/12.3 mm	6.9/14.4 mm	5.9/11.2 mm
Axial resolution:			
- FWHM/FWTM @ x=0 cm, y=1 cm	5.8/n.a. mm	5.3/11.8 mm	5.2/10.8 mm
Scatter fraction:	35%	36%	32%
Total system sensitivity :	17.4 cps/Bq/ml	14.6 cps/Bq/ml	16.1 cps/Bq/ml
True system sensitivity :	12.7 cps/Bq/ml	11.7 cps/Bq/ml	12.1 cps/Bq/ml

Axial sensitivity profile

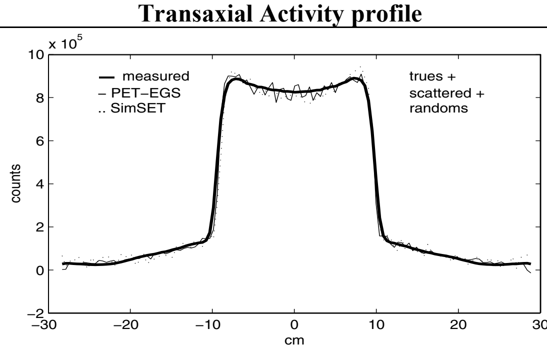


Count rate



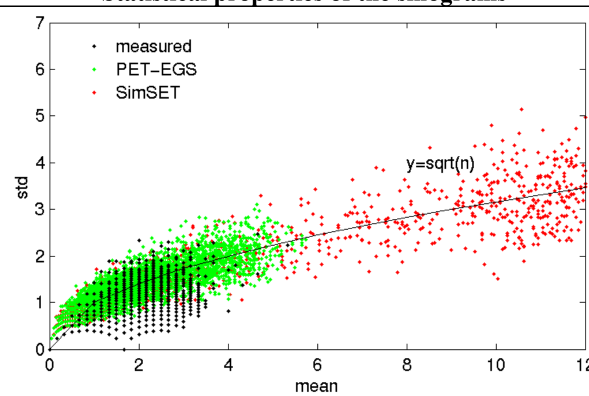
SimSET did not allow simulations of randoms and dead time

Transaxial Activity profile



For SimSET randoms were analytically modeled as a constant background of normally distributed data scaled according to the count rate data.

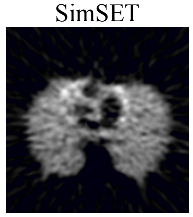
Statistical properties of the sinograms



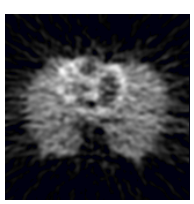
Zubal reconstructed slice

Original

SimSET

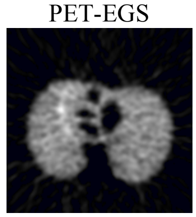


trues

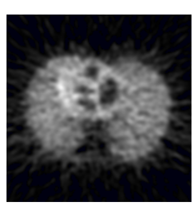


trues + scattered

PET-EGS



trues



trues + scattered

Activity profile through the reconstructed Zubal slice

horizontal

vertical