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RECORDS: improved Reporting of montE CarlO RaDiation transport Studies: Report of the AAPM Research Committee Task Group 268

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Studies involving Monte Carlo simulations are common in both diagnostic and therapy medical physics research, as well as other fields of basic and applied science. As with all experimental studies, the conditions and parameters used for Monte Carlo simulations impact their scope, validity, limitations, and generalizability. Unfortunately, many published peer-reviewed articles involving Monte Carlo simulations do not provide the level of detail needed for the reader to be able to properly assess the quality of the simulations. The American Association of Physicists in Medicine Task Group #268 developed guidelines to improve reporting of Monte Carlo studies in medical physics research. By following these guidelines, manuscripts submitted for peer-review will include a level of relevant detail that will increase the transparency, the ability to reproduce results, and the overall scientific value of these studies. The guidelines include a checklist of the items that should be included in the Methods, Results, and Discussion sections of manuscripts submitted for peer-review. These guidelines do not attempt to replace the journal reviewer, but rather to be a tool during the writing and review process. Given the varied nature of Monte Carlo studies, it is up to the authors and the reviewers to use this checklist appropriately, being conscious of how the different items apply to each particular scenario. It is envisioned that this list will be useful both for authors and for reviewers, to help ensure the adequate description of Monte Carlo studies in the medical physics literature. [https://doi.org/10.1002/mp.12702]

Key words: diagnosis, guidelines, Monte Carlo simulation, publication, radiation transport, radiotherapy

Monte Carlo methods are a powerful alternative to experimental work in many areas of research. As such, the use of Monte Carlo-based computer simulations has become commonplace in both diagnostic and therapy medical physics. The increase in computer power available over the past decades has contributed to the increasing number and complexity of the simulations performed to answer critical questions in our research field. However, as with actual experiments, the design of a Monte Carlo-based computer simulation and selection of its parameter values can result in large variations in the final results, potentially allowing for important biases to be introduced inadvertently. Therefore, judging the appropriateness of a simulation from the description of the methods used in a peer-reviewed article is important, but at the same time increasingly challenging.

In light of this, the American Association of Physicists in Medicine formed Task Group #268 to develop guidelines to improve reporting of Monte Carlo studies in medical physics research. This initiative was inspired by similar guidelines set forth for clinical studies, such as the STARD guidelines for reporting diagnostic studies[1,2] and the CONSORT guidelines for reporting randomized trials,[3,4] among others. The intent of this Task Group was to increase the level of relevant detail of

descriptions used in these studies, which should in turn increase the level of transparency, the ability to reproduce results, and the overall scientific value of these studies. To accomplish this goal, this Task Group developed a checklist of the items that should be included in the Methods, Results and Discussion section of manuscripts submitted for peer review that include Monte Carlo simulations. As such, it is envisioned that this list will be useful both for authors and for reviewers, to help ensure the adequate description of Monte Carlo studies in the medical physics literature. It should be noted that this checklist is drafted so as to be applicable to studies using any Monte Carlo software, both publicly available and developed in-house.

Note, however, that the omission of any of the items listed in the checklist should not be automatically taken as disqualifying. Given the nature of Monte Carlo simulations, there might be scenarios in which some items are either not applicable, are irrelevant, or have no significant impact on the study. Therefore, ultimately it is up to the authors and the reviewers to use this checklist appropriately, being conscious of how the different items apply to each particular study.

It is important to note that it is beyond the scope of this work to specify how Monte Carlo studies should be performed. The correct design, implementation, validation, and performance of a Monte Carlo-based study involve careful consideration of many issues which are usually highly dependent on the application being studied. It is the hope of this Task Group that improving and homogenizing the information provided regarding the study will allow reviewers and readers to better determine its appropriateness, or lack thereof.

In addition to the checklist itself (Table I), the Task Group proposes a template table (Table II) for possible inclusion in the Methods section of manuscripts. The use of this proposed table would allow for the inclusion of many of the checklist items with short phrases and/or references to previous work. The items from Table I that are included in this methodology summary table are denoted with a (*). If Table II is used, the checklist items that are not included in it should be included in text form in the manuscript, in the appropriate sections.

As can be seen in Table I, various items (e.g., variance reduction techniques, statistical uncertainty estimation) include the need to either describe the method or technique used, or to provide references. When a well-documented, public domain Monte Carlo code is used and the referenced method or feature is used with no modification, then software manuals or related publications that provide detailed descriptions of method can be cited, eliminating the need for detailed explanations in the article body. However, if a method was developed or modified by the authors, then a detailed description or reference to previous work should be included.

EXPLANATORY NOTES ON CHECKLIST ITEMS

Items #4 and #17: The extent to which the simulation needs to be validated and the methods used to achieve this will vary considerably depending on the situation. Ideally, experimental validation with conditions representative of those being investigated should be or have been performed, but this is not always feasible or necessary. Replication of previously published results, either experimental or simulations, is often sufficient. For example, where relevant, the AAPM Task Group Report #195 could be used for partial, or where appropriate, complete validation.[5] Reference to previous publications that include the validation(s) performed for the code used and/or description(s) of the new simulation(s) or the experiment(s) performed for validation should be described in the Methods section (Item #4). The results of any new validation efforts should be reported in the table suggested in Table II and/or in the Results section (Item #17). Studies related to simulation efficiency, e.g., presenting new GPU-based code or a new variance reduction technique, in addition to the information listed below regarding timing (Item #5), should include a comprehensive comparison of results against the original code to ensure consistency. This will necessitate the testing with various parameter values.

Item #5: For studies related to simulation efficiency, timing, and/or introduction of a new code or algorithm whose main benefit is increase in computation efficiency, e.g., a new GPU-based Monte Carlo code, then results and timing should be provided for a range of conditions, to better gauge the benefits and limitations of the algorithm presented. It is important to specify how different parameters affect the efficiency. This is especially the case for GPU-based code, where the advantages of parallelization may depend strongly on some simulation parameters in more complex ways than those usually seen for CPU-based code.

For other studies, computation time, at least in order of magnitude, should be specified to provide the readers with an idea of how long such a simulation takes to perform.

Item #6: The composition and geometrical descriptions of some components of a simulated system may be proprietary in nature, and the investigators' access to this information governed by a nondisclosure agreement, precluding its publication. This should not, by itself, compromise the publishability of such studies. However, in some cases it is possible (and if acceptable to the rights holder) to describe proprietary components in terms of equivalent or approximate system characteristics that reproduce the relevant behavior of the proprietary system components. For example, the influence of a proprietary x-ray beam transport system (tube, housing, filters, etc.) may be described in terms of equivalent thickness of aluminum filtration. When available, such equivalent descriptions of proprietary system components should be provided and justified.

Item #7: For simulation geometries that include a voxelized model obtained from computed tomography images, the method to convert from voxel image intensities, e.g., Hounsfield Units, to material composition and density should be described, and a reference provided, if applicable. The voxel size used should be specified. If different voxel sizes are used for geometry specification and for scoring, then all sizes should be specified and the method used to resample should be reported.

Item #8: Information on the source to be provided could include, but not be limited to, type of particle or radiation,

TABLE I. Guidelines for Publications of Monte Carlo Studies: Checklist of the items that should be included in papers in which Monte Carlo calculations are involved. Where possible, items denoted with a (*) may be included in a Methodology table using the template presented in Table II. For items 4 and 5, which have options a and b, depending on the nature of the study, usually only one of the alternatives should be used.

Section and topic	No	Item
Title		
	1	Identification as a Monte Carlo study
Methods		
Software	2*	Name of Monte Carlo software used, including a reference to a paper and/or report describing the package, if available. If the selected code is not commonly used for the application of the current study or if it necessitated considerable modification, then justification for why a certain Monte Carlo code was selected
	3*	Release number and/or release date of Monte Carlo software used
	4a*	If the code has been previously validated or is being validated against previous publications, description of the code's validation in similar or at least relevant applications, preferably via references
	4b*	If code is being validated against experimental measurements, then detailed description of experimental conditions and of simulation study. For the latter, include any assumptions and simplifications of the experimental conditions
Hardware	5a*	If study is related to Monte Carlo efficiency, specification of CPU/GPU time, compiler information, and system used to perform the simulations, including CPU/GPU model number
	5b*	Otherwise specification of order of magnitude of CPU/GPU time and CPU/GPU model number
Geometry	6	Description of simulation geometry, using drawings and tables as needed. Provide all relevant dimensions which are not proprietary and non-disclosable. If possible, provide equivalent composition and dimension information in place of non-disclosable proprietary details
Materials	7	Description of material composition and mass density of each item in the geometry, with references if applicable. Provide the elemental composition and/or, if applicable, the Hounsfield Units conversion method
Source	8*	Description of the source, including: source of phase-space files if used; model used to generate source; and model parameter values. Provide reference, if applicable
Physics and transport	9*	Specification of the cross-section data used along with derived quantities such as stopping powers
	10*	Specification of relevant transport parameters used, such as energy and particle weight cutoffs, step sizes and thresholds. Also transport algorithms if there is more than one option for the code used. Specifying use of the default is adequate if it is unique and documented by citation
	11*	Specification of variance reduction (VRT) and approximate efficiency improvement techniques (AEIT) used, and their parameters. References describing them or specific descriptions of any new techniques should be included if they are not included in the Monte Carlo software as built-in, documented options
Scoring	12*	Specification of the relevant scored quantities. Provide tally names if using a standard Monte Carlo software that includes them, but also include what physical quantity is scored by the tally. When results are binned, tabulated values should make clear what the variable means, e.g., the mid-point, top or range of a bin
	13*	Number of histories and number of source particles used. If various simulations involve different numbers of histories and source particles, at least provide range
	14*	Description and references, as appropriate, of the method used to estimate statistical uncertainty, including if estimated by the history-by-history or the batch method
Analysis	15*	Description of how scored quantities are normalized and/or converted to other metrics. List physical conversion factors used and provide references, if applicable, if there are multiple values for these in the literature
	16*	Description of how scored quantities are de-noised or otherwise filtered, with references, if applicable. If none, then this should be specifically mentioned
Results		
	17*	Results of validation, unless code has been previously validated
	18*	Scored quantities with statistical uncertainty including a specification of the confidence limits used. In general, graphical representation of results such as depth-dose curves or spectra should be histogram rather than point plots, and include uncertainty estimates with error bars in the graphs or text in the caption
Discussion		
	19	Discussion of study limitations, including sources of potential bias, statistical uncertainty, and generalizability
	20	Discussion of assumptions and approximations and their potential effect on the results, given the knowledge gained

shape, energy and its distribution including bin size, and direction, distribution and modulation of emission, etc.

Item #9: Specification of relevant cross-sections used for the simulations should be provided. If the default options of the Monte Carlo simulation code are used, the libraries involved should be listed and referenced. As examples, the following is a short sample of the type of information required, as relevant per the particles and energies involved:

- For low-energy photons (< 200 keV): photoelectric cross-section library. For high atomic number materials, atomic relaxation data source should be referenced.

TABLE II. Template: Monte Carlo methods table: The following table can be completed and included in the Methods section of the paper in lieu of in-line descriptions. This table includes the items of the checklist (Table I) that can often be specified by a short phrase and/or references to previous works (denoted in Table I with a *). The remaining relevant items in Table I should be included in the text of the manuscript.

Checklist item #	Item name	Description	References
2, 3	Code, version/release date		
4, 17	Validation		
5	Timing		
8	Source description		
9	Cross-sections		
10	Transport parameters		
11	VRT and/or AEIT		
12	Scored quantities		
13, 18	# histories/statistical uncertainty		
14	Statistical methods		
15, 16	Postprocessing		

- For kerma approximation and track-length estimators: mass-energy absorption coefficient data source, which should be compatible with cross-sections used for photon transport.
- For x-ray imaging receptor simulations: atomic/molecular form factor data and total linear attenuation coefficient data and inelastic scattering data model used.

Item #10: Data on transport parameters should be provided and referenced, where appropriate. As examples, a short sample of specifications that should possibly be provided are:

- Specify if charged particles are transported.
- Specify transport package used and transport physics used, with references, as appropriate. Providing a reference to the default packages/options used may be enough as long as that is unique for the particular code. Otherwise, values of charged-particle transport parameters should be supplied.
- For response simulations of detectors with gaseous cavities, boundary crossing algorithms should be specified and a relevant Fano cavity benchmarking study referenced.

Item #12: If the scored dose to the medium is being converted to dose to water either on-the-fly or after the simulation, specify the methods used and justify them.

Item #13: Commonly, a history is formed by one primary particle, emitted from the source, and all the secondary particles generated by it. On some occasions, however, it may be convenient to consider several primary particles as forming part of the same history. An example of the latter is when the 1.17 MeV and the 1.33 MeV photons emitted after the disintegration of a Co-60 nucleus are to be considered in conjunction in order to reproduce the sum peak in a spectrometer; here the quantity of interest is the total energy deposited in the spectrometer by both photons and all their descendants. Another example is when using a phase-space source from an accelerator where many particles may correspond to one initial electron. All of these *primary particles* from the phase space are part of the same history. Similarly, if particle splitting is used as a VRT with a phase-space source, all the split particles are part of one history. Given these possible scenarios, when appropriate, listing of both the number of histories and the number of source particles is specified in this Item. That said, the specific number of histories is not as important as the statistical uncertainty on the scored quantities since the number can be meaningless given the effects of VRTs.

Item #15: In most cases, the scored quantity or quantities resulting from the Monte Carlo simulations are normalized to some measurable quantity (often used to experimentally calibrate the system) and might also be converted to a different quantity. For example, in mammographic dosimetry simulations, the resulting energy deposition in the breast tissue might be converted to normalized glandular dose by multiplying by the G factor (the ratio of mass-energy absorption coefficients of glandular tissue to that of the breast tissue mixture) and dividing by the glandular tissue mass and the incident air kerma. The source of these physical values (e.g., mass-energy absorption coefficients, incident air kerma) or the values used (e.g., glandular tissue mass), should be provided. Other examples include correction factors employed for detector response calculations, such as intrinsic energy dependence or other precalculated detector corrections.

Item #16: Smoothing or de-noising algorithms applied to the Monte Carlo simulation results should be specified, along with all relevant algorithm parameters used. If the results are not filtered in any way, then this should be specifically stated.

The use of Monte Carlo simulations in medical physics has become commonplace, and continuing advances in computer power can be expected to only increase the use and complexity of these studies. As with any other studies, Monte Carlo-based simulation studies need to be clearly and comprehensively described to allow for the evaluation of their validity, appropriateness, generalizability and limitations. It is hoped that the guidelines and recommendations in this AAPM Task Group Report will be useful for authors and for reviewers of Monte Carlo-based manuscripts in their efforts.

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CONFLICT OF INTEREST

The authors declare that they do not have any conflict of interest.

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