 DOI: 10.1051/epjconf/201715306008

Recent Improvements of Particle and Heavy Ion Transport code System: PHITS

Tatsuhiko Sato[1,*], *Koji* Niita[2], *Yosuke* Iwamoto[1], *Shintaro* Hashimoto[1], *Tatsuhiko* Ogawa[1], *Takuya* Furuta[1], *Shin-ichiro* Abe[1], *Takeshi* Kai[1], *Norihiro* Matsuda[1], *Keisuke* Okumura[1], *Tetsuya* Kai[1], *Hiroshi* Iwase[3], and *Lembit* Sihver[4]

[1]Nuclear Science and Engineering Center, Japan Atomic Energy Agency, Shirakata, 2-4, Tokai, Ibaraki, 319-1195, Japan
[2]Research Organization for Information Science and Technology, Shirakata, 2-4, Tokai, Ibaraki, 319-1106, Japan
[3]High Energy Accelerator Research Organization, Oho 1-1, Tsukuba, Ibaraki, 305-0801, Japan
[4]Atominstitut, Technische Universität Wien, Stadionallee 2, 1020 Vienna, Austria

Abstract. The Particle and Heavy Ion Transport code System, PHITS, has been developed under the collaboration of several research institutes in Japan and Europe. This system can simulate the transport of most particles with energy levels up to 1 TeV (per nucleon for ion) using different nuclear reaction models and data libraries. More than 2,500 registered researchers and technicians have used this system for various applications such as accelerator design, radiation shielding and protection, medical physics, and space- and geo-sciences. This paper summarizes the physics models and functions recently implemented in PHITS, between versions 2.52 and 2.88, especially those related to source generation useful for simulating brachytherapy and internal exposures of radioisotopes.

1 Introduction

The Monte Carlo particle transport simulation code is an essential tool used in various fields of research such as radiation shielding, radiological protection, and medical physics. We are therefore developing Particle and Heavy Ion Transport code System, PHITS [1], that can simulate the transport of most particles with energy levels up to 1 TeV (per nucleon for ion) by using various nuclear reaction models and data libraries. The system is written in Fortran language and can be compiled using Intel Fortran 11.1 (or later versions) or GFortran (version 4.7 or 4.8). PHITS can be executed on the Windows, Mac, and Linux platforms. Distributed and shared memory parallelization techniques are made available using Message Passing Interface (MPI) protocols and open multi-processing (OpenMP) directives, respectively. Hybrid parallelization using both MPI and OpenMP is also feasible [2]. Various quantities, such as heat deposition, track length, and production yields, can be obtained via PHITS simulation using implemented "tally" estimator functions. Estimation of the time evolution of radioactivity is also feasible using DCHAIN-SP [3], which is also included in the PHITS package.

The latest version of PHITS available from the Organization for Economic Cooperation and

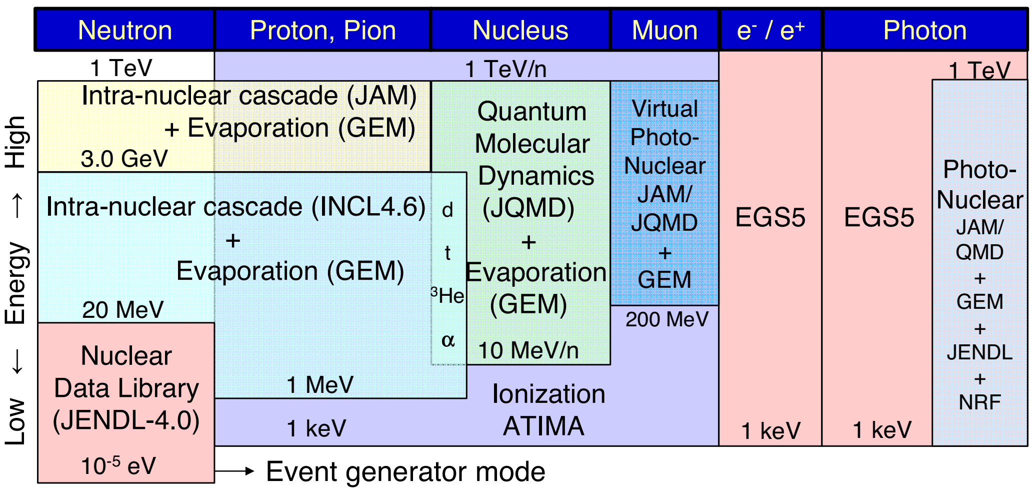

Figure 1. Map of the models and data libraries recommended for use in PHITS 2.88.

* Corresponding author: sato.tatsuhiko@jaea.go.jp

Development/Nuclear Energy Agency (OECD/NEA) databank [4] is 2.82 (Feb. 2016); however, a new version PHITS 2.88 will soon be released. In our previous report, we provided a detailed description of the features and functions of the models before version 2.52, implemented in PHITS [1]. In this paper, a brief summary of the physics models and functions implemented after the earlier mentioned version has been provided, especially those related to source generation for simulating brachytherapy and internal exposure of radioisotopes.

2 New Features

2.1 Upgrades for physics models and libraries

The map of the models and data libraries recommended for use in PHITS 2.88 is shown in Fig. 1. The major upgrades are listed below:

- The maximum energy of the particles that can be handled by PHITS has been extended from 100 GeV to 1 TeV (per nucleon for ions) because of the revisions made to the high energy nuclear reaction models JAM [5] and JQMD [6] as well as the implementation of the EGS5 algorithm [7]. This extension allowed PHITS to be more appropriately utilized in space applications. In addition, the implementation of the EGS5 algorithm improved the accuracy of electron transport simulation particularly for lower energies, which is very important for medical physics applications.
- The JQMD model was further improved to version 2.0, which enables more precise reproduction of the fragmentation cross sections by incorporating the reaction mechanisms that are particularly important for peripheral collisions [8]. Fig. 2 shows the charge changing cross section of 700 MeV/n ^{56}Fe ions incident to a natural carbon target calculated by JQMD and JQMD 2.0 in comparison with the measured data [9]. It is evident from the graph that JQMD 2.0 can reproduce the experimental data very well for high charge fragments, which are predominantly produced by peripheral collisions. This improvement is particularly important for cosmic-ray dosimetry and design of heavy ion therapy.
- The energy ranges of the photonuclear reactions simulated by PHITS were extended up to 1 TeV by implementing the models describing nuclear resonance florescence (NRF) [10] and high-energy photonuclear reactions [11]. The implementation of the NRF model enables the analysis of non-destructive assay of fissile nuclear materials using PHITS.
- The muon transport algorithm was improved by taking into consideration the mechanisms of virtual photonuclear reactions, pair production, bremsstrahlung, and negative muon capture reaction after the formation of a muonic atom [12]. As a benchmark of the newly implemented muon interaction models, underground muon intensities were calculated using PHITS 2.52 and 2.88, and compared with the experimental data [13,14]. The PARMA model [15,16], which was developed based on the airshower simulation performed by PHITS, was used for determining the vertical muon fluxes at the ground level. It can be seen in Fig. 3 that PHITS 2.88 can reproduce the experimental data very well, indicating the accuracy of newly implemented muon interaction models.
- The algorithm for de-excitation of a nucleus after an evaporation process was improved through the implementation of EBITEM [17], enabling precise estimation of γ-ray spectra and isomer production rates. This implementation allows PHITS to be utilized in the prompt γ-ray analysis, which is useful for various purposes such as design of on-line trajectory imaging for charged particle therapy based on gamma cameras.
- The models for calculating the total reaction cross sections were improved [18,19].
- The Kerma factors for some nuclei contained in JENDL-4.0 [20] were revised.
- A new reaction ejectile sampling algorithm to recover kinematic correlations from inclusive cross-section data, so-called event generator mode version 2.0, was

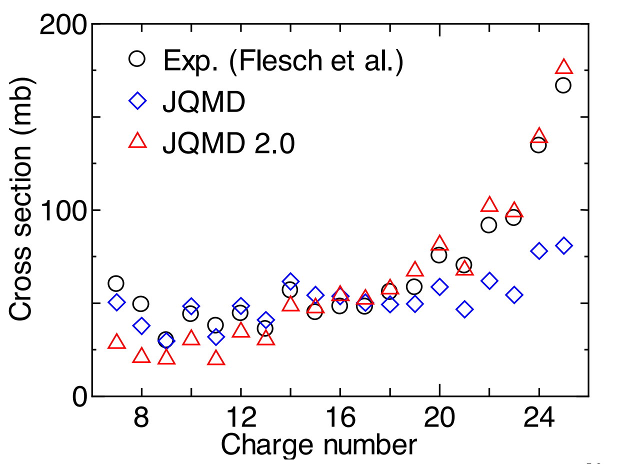

Figure 2. Charge changing cross section of 700 MeV/n ^{56}Fe ions incident to a natural carbon target calculated by JQMD and JQMD 2.0 in comparison with the measured data [9]

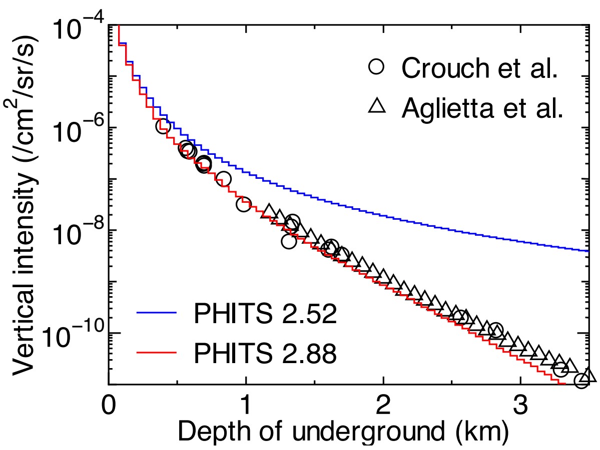

Figure 3. Underground muon intensities calculated using PHITS 2.52 and 2.88 in comparison with the experimental data [13,14]

implemented [21]. The energy spectrum of secondary neutrons and charge particles emitted from low-energy neutron interactions can be precisely determined on the basis of inclusive cross section data such as JENDL-4.0. As an example, the secondary neutron yields from ^{150}Nd(n,2n) reaction induced by 20 MeV neutrons calculated by the event generator mode versions 1 and 2 are shown in Fig. 4. The original inclusive cross section data contained in JENDL-4.0 are also plotted in the graph. The figure clearly indicates that the new version can reproduce the original data very well. This improvement enables more precise calculations of detector responses and dose equivalents due to neutron exposure below 20 MeV.

- DCHAIN-SP was improved by expanding the number of energy groups in its neutron-activation cross section libraries.
- A new approach for describing (d,xn) spectra at energies below 50 MeV was developed in combination with the intra-nuclear cascade model and the Distorted Wave Born Approximation (DWBA) [22]. Fig. 5 shows the double differential cross section of neutrons produced from natural lithium target bombarded by 40 MeV deuteron calculated by Intra-Nuclear Cascade of Liège (INCL) [23] coupled with and without DWBA. The corresponding experimental data [24] are also plotted in the graph. It is evident from the figure that the peaks observed over 40 MeV can be reproduced only by INCL with DWBA because such high-energy peaks are formed due to the discrete levels of nuclear structure, which can be considered only in DWBA. This improvement allows PHITS to be utilized in the design of neutron sources based on deuteron accelerators such as International Fusion Materials Irradiation Facility (IFMIF) project.
- The computational speed of ATIMA [25] in PHITS was improved to allow for the selection of ATIMA as the default stopping power calculation model.

2.2 Upgrades for support functions

In addition to the above-mentioned upgrades to the physics models and libraries, several user support functions were implemented for extending the capabilities of PHITS. The following list describes newly introduced functions in ver. 2.88, and the details of each are described in the PHITS manual [26]:

- The ability to read tetrahedral geometry (a kind of polygonal geometry) was implemented.
- The resolution of a detector can be taken into account when calculating the pulse-height tally.
- The statistical uncertainties in the results of tallies can be properly calculated even when the successive calculation mode using "dump" source.
- The absorbed dose in the unit of Gy can be calculated by considering the mass of the tally regions.
- A new tally for calculating the particle fluence at certain points, so-called the point estimator, was implemented.
- Particle fluxes can be calculated in the cylindrical co-ordinate as a function of the azimuth angle.
- Several user support functions were developed and introduced, including those for visualizing geometry errors, summing up two (or more) tally results, and defining a user's original tally.
- A conversion program from the DICOM image data to the PHITS input format, DICOM2PHITS, was developed.
- A function to automatically determine the appropriate weight windows (weight window generator) was implemented.
- A function that outputs PHITS tally results into a format usable by ParaView [27], which is an open-source, multi-platform data analysis and visualization application, was developed. For example, Fig. 6 shows the ParaView visualization of the absorbed doses in skeletal tissue of the International Commission on Radiological Protection (ICRP) adult male phantom [28] that has been irradiated by 1 GeV proton in the PHITS simulation.

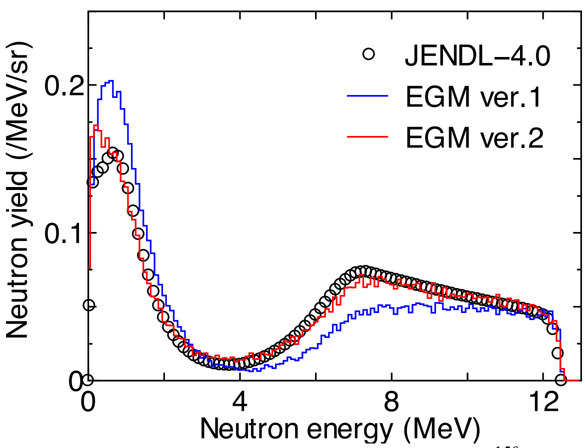

Figure 4. Secondary neutron yields from ^{150}Nd(n,2n) reaction induced by 20 MeV neutrons calculated by the event generator mode (EGM) versions 1 and 2, in comparison with the original inclusive cross section data contained in JENDL-4.0 [20]

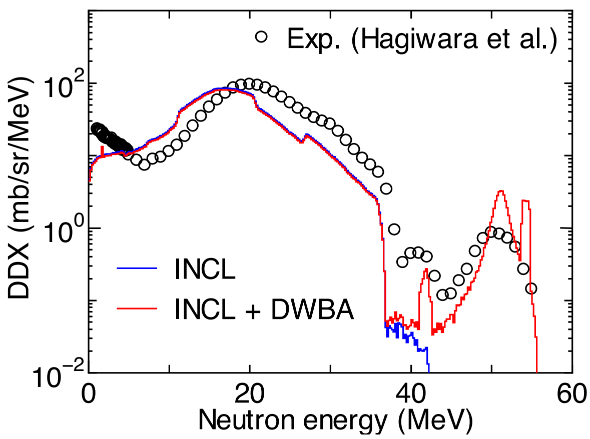

Figure 5. Double differential cross section of neutrons produced from natural lithium target bombarded by 40 MeV deuteron calculated by Intra-Nuclear Cascade of Liège (INCL) coupled with and without DWBA in comparison with the corresponding experimental data [24]

2.3 Upgrades for source generation

Recently, PHITS has been used for estimating the risk of internal exposure of radioisotopes [29] and therapeutic effects of brachytherapy on the basis of microdosimetric simulations. To conduct such simulations using the earlier versions of PHITS, the energy and emission probability of the radiations generated per nuclear transformation of radioisotopes were required to be specified by users by investigating the nuclear decay data such as level structure and branching ratios. However, it is sometimes difficult to evaluate the source term, particularly when the daughter nuclides of the radioisotopes are also radioactive.

Therefore, we developed a new source generation function that can automatically determine the discrete γ-ray spectra emitted from the decay of radioisotopes, including the contributions made by their daughter nuclides. The nuclear-decay data files for dose calculation, DECDC [30], which is equivalent to that in the database contained in ICRP Publication 107 [31], is employed as reference data for this new function. The input parameters to be specified in this function are the name and activity (Bq) of the initially existing radioisotopes and the time for the calculation of the activities after considering their decay chains. Fig. 7 shows the photon fluxes emitted one year after the decay of ^{144}Ce, which had had an initial activity of 100 Bq. Not only low-energy photons emitted from ^{144}Ce but also high-energy photons emitted from its daughter nuclides, such as ^{144}Pr and ^{144m}Pr, can be observed in the spectrum. Only the photon emission function can be dealt currently using this function; however, we intend to extend this functionality to enable handling of electron and alpha emissions as well.

It is occasionally required to consider the correlation of source particles for the exact reproduction of the internal exposure situations because some radioisotopes emit two (or more) radiations at once. Therefore, we have developed a function that generates multiple particles as an event while considering their angular correlation. This function is particularly important for simulating the microdosimetric profile of boron neutron capture therapy, because an α particle and a ^{7}Li ion are generated from the same location but opposite directions during a ^{10}B(n,α)^{7}Li reaction.

We also implemented source generation functions for reproduction of spontaneous fission neutrons [32] and reading of International Atomic Energy Agency (IAEA) phase space files [33]. The former is useful for simulations of radiological protection of internal exposure of spontaneous fission nuclides [34], whereas the latter is beneficial for medical physics simulations of X-ray therapy.

3 Conclusions

PHITS has been used in many countries for various applications, such as accelerator design, radiation shielding and protection, medical physics, and space- and geo-sciences. The tutorials of the code are organized several times per year in Japan, and sometimes in other countries such as France and Malaysia. Owing to the continuous improvement and promotion of the code, the number of registered users exceeded 2,500 in 2016, and has been rapidly increasing since then. A comprehensive benchmark calculation results of the new version of PHITS will be published elsewhere [35].

Acknowledgements

We are grateful for the support of Center for Computational Science & e-Systems (CCSE) of JAEA in promoting PHITS. We wish to thank Dr. Y. Namito and Dr. H. Hirayama of KEK for their advice in implementing the EGS5 algorithm. We would also like to thank Dr. Y. Mizuno of Kyoto Women's University for his advice in implementing the muon reaction models, Dr. L. Pong Hong of NAIS Co. Ltd. for his support in developing the function for generating fission neutron sources, and Mr. M. Adachi, Mr. T. Miura, and Mr. A. Wada of RIST for their assistance in the programing of PHITS. The function to read tetrahedral geometry was implemented under the support of Hanyang University Radiation Engineering Laboratory (HUREL), Korea. The function for tally results output in ParaView format was majorly programmed at

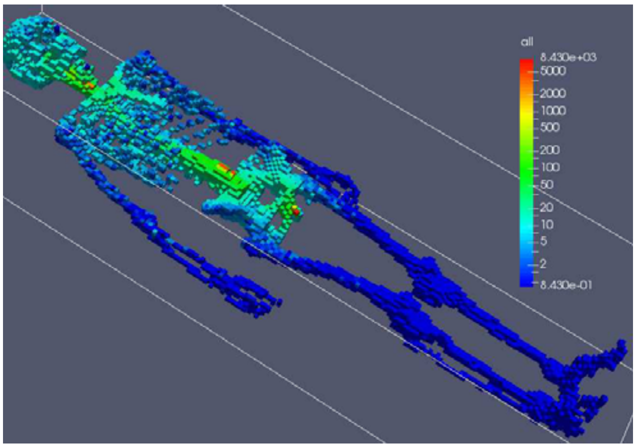

Figure 6. ParaView visualization of absorbed doses in the skeletal tissue of the ICRP adult male phantom that has been irradiated by 1 GeV proton in the PHITS simulation

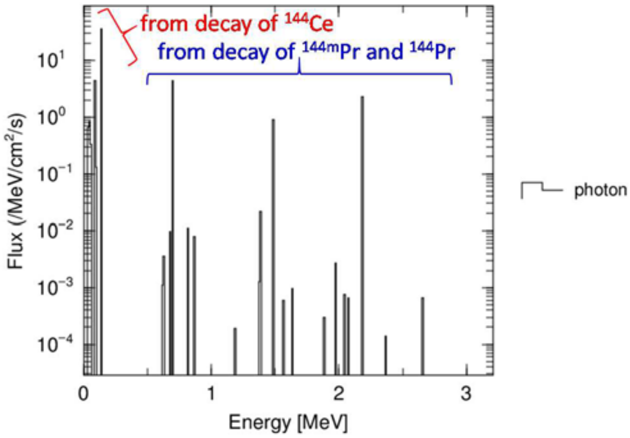

Figure 7. Photon fluxes emitted after one year of decay of ^{144}Ce with an initial activity of 100 Bq. The fluxes were obtained 1 cm away from the source location.

Visible Information Center, Inc. This work is partially supported by Japan Society for the Promotion of Science (JSPS), Grant-in-Aid for Scientific Research (C), Grant Number JP26461900.

References

1. T. Sato, K. Niita, N. Matsuda, S. Hashimoto, Y. Iwamoto, S. Noda, T. Ogawa, H. Iwase, H. Nakashima, T. Fukahori, K. Okumura, T. Kai, S. Chiba, T. Furuta and L. Sihver, Particle and Heavy Ion Transport Code System PHITS, Version 2.52, J. Nucl. Sci. Technol. **50**, 913-923 (2013).
2. T. Furuta, K.L. Ishikawa, N. Fukunishi, S. Noda, S. Takagi, T. Maeyama, K. Fukasaku, and R. Himeno, *Implementation of OpenMP and MPI hybrid parallelization to Monte Carlo dose simulation for particle therapy*, IFMBE Proceedings, **39**, 2099-2102. (2012).
3. T. Kai, F. Maekawa, K. Kosako, Y. Kasugai, H. Takada, and Y. Ikeda, *DCHAIN-SP 2001: High energy particle induced radioactivity calculation code*, JAERI-Data/Code 2001-016, (2001). [in Japanese]
4. http://www.oecd-nea.org/tools/abstract/detail/nea-1857/
5. Y. Nara, H. Otuka, A. Ohnishi, K. Niita, and S. Chiba, Relativistic nuclear collisions at 10A GeV energies from p+Be to Au+Au with the hadronic cascade model, Phys. Rev. C **61**, 024901 (2000).
6. K. Niita, S. Chiba, T. Maruyama, T. Maruyama, H. Takada, T. Fukahori, Y. Nakahara, and A. Iwamoto, Analysis of the (N,Xn') Reactions by Quantum Molecular-Dynamics Plus Statistical Decay Model, Phys. Rev. C **52**, 2620-2635 (1995).
7. H. Hirayama, Y. Namito, A.F. Bielajew, S.J. Wilderman, and W.R. Nelson, *The EGS5 code system*, SLAC-R-730 and KEK Report 2005-8, (2005).
8. T. Ogawa, T. Sato, S. Hashimoto, D. Satoh, S. Tsuda, and K. Niita, Energy-dependent fragmentation cross sections of relativistic ^{12}C, Phys. Rev. C **92**, 024614 (2015).
9. F. Flesch, S.E. Hirzebruch, G. Hüntrup, H. Röcher, T. Streibel, E. Winkel, W. Heinrich, Fragmentation cross section measurements of iron projectiles using CR-39 plastic nuclear track detectors, Radiat. Meas., **31**, 533-536 (1999)
10. T. Ogawa, S. Hashimoto, T. Sato, Development of general nuclear resonance fluorescence model, J. Nucl. Sci. Technol. **53**, 1766-1773 (2016).
11. S. Noda, S. Hashimoto, T. Sato, T. Fukahori, S. Chiba and K. Niita, Improvement of photonuclear reaction model below 140 MeV in the PHITS code, J. Nucl. Sci. Technol. **52**, 57-62 (2015).
12. S. Abe and T. Sato, Muon interaction models implemented into PHITS. J Nucl Sci Technol. **53**, 451-458 (2016).
13. M. Crouch, An improved world survey expression for cosmic ray vertical intensity vs. depth in standard rock, Proc. 20th Int. Cosmic Ray Conf.; 1987 Aug 2-15; Moscow (USSR). **6**, 165-168 (1987).
14. M. Aglietta, B. Alpat, E. D. Alyea et al., Muon "depth-intensity" relation measured by the LVD underground experiment and cosmic-ray muon spectrum at sea level, Phys. Rev. D. **58**, 092005 (1998).
15. T. Sato, Analytical Model for Estimating Terrestrial Cosmic Ray Fluxes Nearly Anytime and Anywhere in the World: Extension of PARMA/EXPACS, PLOS ONE **10**(12), e0144679 (2015).
16. T. Sato, Analytical Model for Estimating the Zenith Angle Dependence of Terrestrial Cosmic Ray Fluxes. PLOS ONE **11**(8): e0160390 (2016).
17. T. Ogawa, S. Hashimoto, T. Sato, K. Niita, Development of gamma de-excitation model for prediction of prompt gamma-rays and isomer production based on energy-dependent level structure treatment, Nucl. Instr. Meth. B 325, 35-42 (2014).
18. L. Sihver, A. Kohama, K. Iida, K. Oyamatsu, S. Hashimoto, H. Iwase, K. Niita, Current status of the "Hybrid Kurotama model" for total reaction cross sections, Nucl. Instr. Meth. B **334**, 34-39 (2014).
19. T. Sato, R. Kataoka, H. Yasuda, S. Yashiro, T. Kuwabara, D. Shiota and Y. Kubo, Air Shower Simulation for WASAVIES: Warning System for Aviation Exposure to Solar Energetic Particles, Radiat. Prot. Dosim. **161**, 274-278 (2014).
20. K. Shibata, O. Iwamoto, T. Nakagawa, N. Iwamoto, A. Ichihara, S. Kunieda, S. Chiba, K. Furutaka, N. Otuka, T. Ohsawa, T. Murata, H. Matsunobu, A. Zukeran, S. Kamada, and J. Katakura, JENDL-4.0: A New Library for Nuclear Science and Engineering, J. Nucl. Sci. Technol. **48**, 1-30 (2011).
21. T. Ogawa, T. Sato, S. Hashimoto, K. Niita, Development of a reaction ejectile sampling algorithm to recover kinematic correlations from inclusive cross-section data in Monte-Carlo particle transport simulations, Nucl. Instr. Meth. A **763**, 575-590 (2014).
22. S. Hashimoto, Y. Iwamoto, T. Sato, K. Niita, A. Boudard, J. Cugnon, J.C. David, S. Leray, D. Mancusi, New approach to description of (*d*,*xn*) spectra at energies below 50 MeV in Monte Carlo simulation by intra-nuclear cascade code with Distorted Wave Born Approximation, Nucl. Instr. Meth. B **333**, 27-41 (2014).
23. A. Boudard, J. Cugnon, J.C. David, S. Leray, and D. Mancusi, New potentialities of the Liège intranuclear cascade model for reactions induced by nucleons and light charged particles, Phys. Rev. C **87**, 014606 (2013).
24. M. Hagiwara, T. Itoga, N. Kawata, N. Hirabayashi, T. Oishi, T. Yamauchi, M. Baba, M. Sugimoto, and T. Muroga, Measurement of neutron emission spectra in Li(*d*,*xn*) reaction with thick and thin targets for 40-MeV deuterons, Fusion Sci. Technol. **48**, 1320-1328 (2005).
25. https://web-docs.gsi.de/~weick/atima/
26. http://phits.jaea.go.jp/manual/manualE-phits.pdf
27. http://www.paraview.org
28. International Commission on Radiological Protection, *Adult reference computational phantoms*, ICRP Publication 110, Ann ICRP **39**(2) (2009).

29. T. Sato, K. Manabe, N. Hamada, Microdosimetric analysis confirms similar biological effectiveness of external exposure to gamma-rays and internal exposure to ^{137}Cs, ^{134}Cs, and ^{131}I, PLOS ONE **9**(6), e99831 (2014).
30. A. Endo, Y. Yamaguchi and K.F. Eckerman, *Nuclear decay data for dosimetry calculation - Revised data of ICRP Publication 38*, JAERI 1347 (2005).
31. International Commission on Radiological Protection, *Nuclear decay data for dosimetric calculations*, ICRP Publication 107, Ann ICRP **38**(3) (2008).
32. J.M. Verbeke, C. Hagmnn, and D. Wright, *Simulation of neutron and gamma ray emission from fission and photofission*, UCRL-AR-228518 (2014).
33. https://www-nds.iaea.org/phsp/
34. A. Endo and T. Sato, Analysis of Linear Energy Transfers and Quality Factors of Charged Particles Produced by Spontaneous Fission Neutrons from ^{252}Cf and ^{244}Pu in the Human Body, Radiat. Prot. Dosim. **154**, 142-147 (2013).
35. Y. Iwamoto, T. Sato, S. Hashimoto, T. Ogawa, T. Furuta, S. Abe, T. Kai, N. Matsuda, R. Hosoyamada, and K. Niita, Comprehensive benchmark study for the recent version of the PHITS code, *submitted*.