VALIDATION OF SERPENT FOR FUSION NEUTRONICS ANALYSIS AT JET

Andrej Žohar^{1,2}, Žiga Štancar¹, Paola Batistoni^{3,4}, Sean Conroy⁵, Luka Snoj^{1,2}, Igor Lengar¹ and JET contributors⁶

¹Reactor Physics Department, Jožef Stefan Institute Jamova cesta 39, 1000 Ljubljana, Slovenia

²University of Ljubljana, Faculty of Mathematics and Physics Jamova cesta 19, 1000 Ljubljana, Slovenia

> ³Fusion Technical Unit Via E. Fermi 45, I-00044 Frascati, Italy

⁴CCFE, Culham Science Center Abingdon, OX14 3DB, UK

⁵VR, Department of Physics and Astronomy, Uppsala University Box 516, SE-75120 Uppsala, Sweden

⁶See the author list of E. Joffrin et al. accepted for publication in Nuclear Fusion Special issue 2019, https://doi.org/10.1088/1741-4326/ab2276

andrej.zohar@ijs.si, ziga.stancar@ijs.si, paola.batistoni@enea.it, sean.conroy@physics.uu.se, luka.snoj@ijs.si, igor.lengar@ijs.si

ABSTRACT

Fusion neutronics analysis before and after experiments at JET is traditionally performed using Monte Carlo particle transport code Monte Carlo N-Particle. For redundancy and diversity reasons there is a need of an additional Monte Carlo code, such as Serpent 2, capable of fusion neutronics analysis. In order to validate the Serpent code for fusion applications a detailed model of JET was used. Neutron fluxes and reaction rates were calculated and compared for positions outside the tokamak vacuum vessel, in the vacuum vessel above the plasma and next to a limiter inside the vacuum vessel. For all detector positions with DD and DT neutron sources the difference between neutron fluxes calculated with both Monte Carlo codes were within 2σ statistical uncertainty and for most positions (more than 90 % of all studied positions) even within 1σ uncertainty. Fusion neutronics analysis in the JET tokamak with Serpent took on average 10 % longer but this can be improved by changing the threshold value for determination of the transport method used. With the work presented in this paper the Serpent Monte Carlo code was validated to be a viable alternative to MCNP for fusion neutronics analysis for the JET tokamak.

KEYWORDS: Neutron transport, MCNP, Serpent, JET

1. INTRODUCTION

Fusion neutronics analysis performed before and after experiments at JET are commonly supported by neutron transport calculations with the Monte Carlo particle transport code Monte Carlo N-Particle (MCNP)[1]. For fusion devices under design or construction, e.g., ITER and DEMO, the neutronics analysis for design and licensing is also performed by using MCNP. Complex Monte Carlo models are needed to obtain accurate results for verification of experiments and analysis of proposed designs. For the JET tokamak the current MCNP model has approximatly 4 000 cells and surfaces while the reference model for ITER (C-Model) has approximately 100 000 cells and surfaces [2].

MCNP is a neutron transport code of US origin distributed through Radiation Safety Information Computational Centre. Its distribution is controlled, limited and subjected to US regulation. For this reason there is a need of an additional Monte Carlo code capable of fusion neutronics analysis for redundancy and diversity. Monte Carlo code Serpent 2 was first developed for nuclear analysis in fission reactors and burnup calculations and is under consideration as an alternative to MCNP for fusion neutronic analysis as it recently received several enhancements (coupled neutron-photon transport, variance reduction methods, etc.) that make it viable for use in fusion neutronics analysis and is easily obtainable through OECD/NEA [3].

The validation of Serpent for fusion neutronics analysis has been divided into two steps. In the first step the code validation was performed on a representative simplified model of a fusion tokamak reactor to study the effects of material cross sections on neutron transport and effects of neutron transport parameters (e.g. mean distance for the collision flux estimator, threshold for delta-tracking, etc.) and source definition on results. The results of the performed analysis are presented in [4]. In the second step, presented in this paper, the code was validated on a detailed model of the tokamak JET.

The paper is organized as follows. In the first section the detailed MCNP model of the JET tokamak is presented and the process of converting it to Serpent. Second section presents the process of constructing a realistic plasma neutron source in Serpent on the basis of the neutron source used with MCNP. The last part of the paper presents the comparison of results between MCNP and Serpent at different in-vessel and ex-vessel detector positions for validation of Serpent for fusion neutronics analysis. An analysis of the transport parameter dt in Serpent, defining the threshold for delta-tracking transport method, was also performed.

2. SERPENT 2

The Serpent code, released in 2009, was first developed for nuclear analysis in fission reactors and burnup calculations. The current version, Serpent 2, has received several enhancements that make it viable for Monte Carlo calculations beyond fission reactors. Serpent 2 now supports coupled neutron-photon transport, variance reduction methods, direct equivalents to most of the surface types contained in MCNP, cell and mesh tallies, ENDF reaction rate tally multipliers, custom response functions, etc. [5].

A significant difference between MCNP and Serpent is in the implementation of particle transport. MCNP uses the surface-to-surface tracking method for particle transport over cell and material boundaries while Serpent uses a combination of surface-to-surface tracking method and Woodcock delta tracking method [4,6]. The Woodcock delta tracking method allows for faster transport of particles in complex geometries by homogenizing the material total cross sections in such a way, that the sampled path lengths are valid over the entire geometry. This is achieved with the use of a majorant cross section for path length determination. The majorant cross section is the highest total cross section in the entire simulated model. This allows the random walk of particles to continue across material boundaries thus speeding up the particle random walk in complex geometries. However, the method also has disadvantages for fusion applications. Due to characteristics of the method the track length estimator cannot be used for calculation of fluxes and a less efficient collision flux estimator always yields a zero result. To overcome this disadvantages Serpent uses a combination of both methods for particle transport and the threshold value that expresses the ratio between material cross section and majorant cross section, is used for determination of the tracking method.

2.1. JET Monte Carlo model

The majority of neutronics analysis performed before and after experiments at JET is performed using MCNP. Due to this a detailed model of the tokamak structure and surrounding diagnostic equipment already exists. The model is composed of around 4 000 cells and surfaces and has been validated on several different experiments performed in the past. The model is depicted in Fig.1. As Serpent has direct equivalents to most of the MCNP surfaces the model was rewritten to Serpent. This was achieved with an existing script for conversion of MCNP models to Serpent which was tested with a simplified tokamak model [4]. It was ensured no errors occurred in the model by ensuring no cell overlapped another cell and that during the computation neutrons were not lost due to errors in geometry. The position of cells in the model was verified by plotting the Serpent model geometry and comparing it to MCNP geometry plots.



Figure 1: Cross sectional view of the JET tokamak model. The horizontal section is presented in (a) and the vertical section is presented in (b).

2.2. Neutron source

Neutron analysis for support of JET experiments is performed with a D shaped neutron source modelled on basis of several discharges at JET. The position and shape of the neutron source is presented in Fig.2. The highest emission of neutrons is in the centre of the plasma and decreasing towards the edge of plasma. The neutron source in MCNP is defined as a combination of toroidal rings in vertical cross section with different probability of neutron emission but uniform distribution in the toroidal angle and isotropic distribution in the angle of neutron birth. The neutron energy is sampled from a Gaussian distribution with mean energies of 2.5 MeV in deuterium-deuterium plasma (DD) and 14.1 MeV in deuterium-tritium plasma (DT). The source definition in MCNP was rewritten to Serpent. At the time of rewriting the neutron source Serpent did not have the capability to sample neutrons over cylindrical geometry. Due to this the neutron source from MCNP was rewritten as a user defined source in Serpent. The constructed neutron source was validated on a simplified tokamak model [4].



Figure 2: Sectional view of a realistic D shaped neutron source used for comparison between MCNP and Serpent. The highest neutron emission is in the centre of the plasma (yellow region) and is decreasing towards the plasma edge (blue regions).

3. RESULTS OF VALIDATION

For the computations it was ensured that the same material isotopic composition, the same nuclear data library, namely FENDL-3.1d [7], and the same neutron source was used in both Monte Carlo codes. The neutron fluxes were calculated in the positions of three fission chambers called KN1 located outside the vacuum vessel next to the transformer limbs (Fig.1), in four indium foils located in irradiation ends, called KN2-3U, located above plasma on the inside of the vacuum vessel commonly used for neutron activation measurements (Fig.1) and in a long term irradiation station called I-LTIS located inside the vacuum vessel next to a limiter (Fig.1). For the indium foils located in the KN2-3U position the reaction rates were also calculated as the activation of foils is used for absolute calibration of JET neutron detectors, i.e. the KN1 fission chambers. The results of comparison between Serpent and MCNP calculated neutron fluxes and reaction rates are

presented in Fig.3 and Fig.4.

For the KN1 fission chamber positions the calculated neutron fluxes show good agreement as the difference between Serpent and MCNP is less than 0.3 % for DD and DT plasmas while the statistical uncertainty of MCNP and Serpent is 0.4 %. The difference in the calculated neutron fluxes and reaction rates for Indium-115 between Serpent and MCNP for KN2-3U position is larger for DD plasma at around 0.8 % while for DT plasma the difference is less than 0.2 %. The uncertainties of calculated neutron fluxes with MCNP and Serpent for KN1 and KN2-3U were 0.8 % while uncertainties of reaction rates were 1.5 %. The highest difference between MCNP and Serpent can be observed for the calculated neutron fluxes in the long-term irradiation station I-LTIS. The irradiation station consists of 30 positions for samples with diameter of $1.8 \,\mathrm{cm}$ and thickness of 2 mm. The statistical uncertainty of the calculated neutron fluxes with MCNP is 0.6% for all irradiation locations and the variation of neutron fluxes between positions is around 2% despite close clustering of positions. For neutron fluxes calculated with Serpent the statistical uncertainties are around 5 % and the variation of neutron fluxes between positions is around 6 %. The current results show good agreement between MCNP and Serpent for calculation of neutron fluxes in detector positions located outside the vacuum vessel and close to plasma, but there are still observable differences for small detector positions close to the plasma and inside the vacuum vessel.

An important parameter for viability of Serpent for fusion neutronics is also the computational time. For all studied cases the computational time of Serpent was slower compared to MCNP by around 10 %.



Figure 3: Relative difference of neutron fluxes between Serpent and MCNP for all detector positions and reaction rates in a DD plasma. The 1σ uncertainty of MCNP is presented with the green bars while the 1σ uncertainty of Serpent is presented with lines.



Figure 4: Relative difference of neutron fluxes between Serpent and MCNP for all detector position and reaction rates in DT plasma. The 1σ uncertainty of MCNP is presented with the green bars while the 1σ uncertainty of Serpent is presented with lines.

3.1. Analysis of dt parameter

As already stated in the paper Serpent uses two different methods for neutron transport, namely surface-to-surface and delta tracking method. The parameter determining which method is used for neutron transport is called dt. The parameter is one minus the ratio of the total cross section in the material the particle is located in and the majorant (dt = $1 - \frac{\Sigma_{T,i}}{\Sigma_M}$), or in other words the parameter dt represents the size of the interval for usage of the delta tracking method. By default the value of the parameter is set at 0.9, i.e. delta tracking is used if the ratio between the total cross section and the majorant is above 0.1. If the value of parameter is 1 only delta tracking method is used. All previously presented results used the default threshold value for determination of the transport method.

To analyse the effectiveness of delta tracking method for fusion neutronics analysis the parameter dt was varied from 0 to 0.9, i.e. from only surface-to-surface tracking method to default parameter. For all values of parameter dt the calculated neutron fluxes and reaction rates for all positions were within statistical uncertainty compared to MCNP thus proving that the particle transport method does not affect results. However, the calculation times differed depending on the value of parameter dt. The relative difference in computation time between Serpent and MCNP for different values of parameter dt are presented in Fig.5. The results presented are for DD plasma only but results for a DT plasma are similar.

The results show that computational time of Serpent is similar to MCNP for only surface-to-surface tracking method. With the default value of parameter dt the computational time of Serpent is slower by 10 % compared to MCNP. This is due to the use of delta tracking method in majority of materials. By the lowering of the size of the interval the number of materials and regions in which surface-to-surface tracking method is used increases. As there are many and big regions in the JET tokamak model with low total cross section (e.g. air surrounding the tokamak) the particle transport is faster with the surface-to-surface tracking method. This is opposite to situation in fission reactors where the delta tracking method can speed up computation time compared to MCNP. Due to this it is recommended to lower the threshold value of parameter dt for fusion neutronics analysis to obtain similar computing time in Serpent and MCNP.



Figure 5: Relative difference in computational time of Serpent to MCNP for different threshold values of parameter dt for determination of used transport method. The results presented are only for a DD plasma but the results are similar for a DT plasma.

4. CONCLUSIONS

In this paper an analysis of the Serpent Monte Carlo code was performed for its use in fusion neutronics analysis for the JET tokamak. During the analysis it was ensured: the same tokamak model, the same material compositions, the same evaluated nuclear data libraries and the same neutron sources in Serpent and the reference code MCNP were used. A D shaped neutron source in Serpent was modelled to be representative of high performance discharges at JET. It was rewritten to Serpent as a user defined source as at the time of the analysis Serpent did not support the same source definitions as MCNP.

The comparison of calculated neutron fluxes between MCNP and Serpent was performed for three fission chamber positions called KN1 located outside the tokamak vacuum vessel, in activation system named KN2-3U on top of plasma in the vacuum vessel structure and long term irradiation station I-LTIS next to a limiter inside the vacuum vessel. For all detector positions with the DD and

DT neutron sources the difference between neutron fluxes calculated with MCNP and Serpent were within 2σ Monte Carlo statistical uncertainty and for most positions even within 1σ uncertainty. For reaction rates in In-115 at the position KN2-3U the calculated values between Serpent and MCNP are within 1σ statistical uncertainty. There are significant differences between Serpent and MCNP for fusion neutronics analysis in small regions, like the sample positions in I-LTIS, where Serpent has a lower efficiency thus producing results with higher statistical uncertainty compared to MCNP for the same number of simulated particles.

Serpent uses two different methods for neutron transport - surface-to-surface and delta tracking. By default the surface-to-surface tracking method is only used when the ratio between the material total cross section and the majorant cross section is below 0.1. For fusion neutronics analysis in the JET tokamak this threshold value needs to be increased with the parameter dt as this speeds up the computation to the same computing time as MCNP.

With the presented results the Serpent Monte Carlo code was validated to be a viable alternative to MCNP for fusion neutronics analysis at the JET tokamak.

ACKNOWLEDGEMENTS

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

The work was supported by the Slovenian Ministry of Education, Science and Sport (projects codes: P2-0073 Reactor Physics; P2-0405 Fusion technologies; 1000-17-0106-6 - Training of young researchers).

REFERENCES

- [1] C. J. Werner. *MCNP Users Manual Code Version 6.2*. Los Alamos National Laboratory, report LA-UR-17-29981 (2017).
- [2] D. Leichtle et al. "The ITER tokamak neutronics reference model C-Model." *Fusion Engineering and Design*, **volume 136**, pp. 742 746 (2018). Special Issue: Proceedings of the 13th International Symposium on Fusion Nuclear Technology (ISFNT-13).
- [3] J. Leppänen et al. "The Serpent Monte Carlo code: Status, development and applications in 2013." *Annals of Nuclear Energy*, **volume 82**, pp. 142 150 (2015).
- [4] A. Žohar, I. Lengar, and L. Snoj. "Comparison of MCNP and Serpent for Fusion Transport Simulations." In *Proceedings*, 28th International Conference Nuclear Energy for New Europe NENE 2019 (2019).
- [5] A. Turner et al. "Applications of Serpent 2 Monte Carlo Code to ITER Neutronics Analysis." *Fusion Science and Technology*, **volume 74**(4), pp. 315–320 (2018).
- [6] J. Leppänen. "Performance of Woodcock delta-tracking in lattice physics applications using the Serpent Monte Carlo reactor physics burnup calculation code." *Annals of Nuclear Energy*, volume 37(5), pp. 715 – 722 (2010).
- [7] A. Koning and A. Trkov. "FENDL-3.1d: Fusion Evaluated Nuclear Data Library Ver.3.1d." (2018). URL https://www-nds.iaea.org/fendl/.