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Applications of Serpent 2 Monte Carlo Code to ITER Neutronics Analysis

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Abstract — *Nuclear analysis supporting the design and licensing of ITER is traditionally performed using MCNP and the reference model C-Model; however, the complexity of C-Model has resulted in the geometry creation and integration process becoming increasingly time-consuming. Serpent 2 is still a beta code; however, recent enhancements mean that it could, in principle, be applied to ITER neutronics analysis. Investigations have been undertaken into the effectiveness of Serpent for ITER neutronics analysis and whether this might offer an efficient modeling environment.*

An automated MCNP-to-Serpent model conversion tool was developed and successfully used to create a Serpent 2 variant of C-Model. A version of the deuterium-tritium plasma neutron source was also created. Standard reference tallies in C-Model for the blanket and vacuum vessel heating were implemented, and comparisons were made between the two transport codes assessing nuclear responses and computer requirements in the ITER model. Excellent agreement was found between the two codes when comparing neutron and photon flux and heating in the ITER blanket modules and vacuum vessel.

Comparing tally figures of merit, computer requirements for Serpent were typically three to five times that of MCNP, and memory requirements were broadly similar. While Serpent was slower than MCNP when applied to fusion neutronics, future developments may improve this, and Serpent offers clear benefits that will reduce analyst time, including support for meshed geometry, robust universe implementation that avoids geometry errors at the boundaries, and mixed geometry types. Additional work is proceeding to compare Serpent against experiment benchmarks relevant for fusion shielding problems. While further developments are needed to improve variance reduction techniques and reduce simulation times, this paper demonstrates the suitability of Serpent to some aspects of ITER analysis.

Keywords — *Neutronics, Serpent, ITER.*

Note — *Some figures may be in color only in the electronic version.*

I. INTRODUCTION

Nuclear analysis is required to support the successful design of ITER, traditionally performed using MCNP (Ref. 1) with a neutronics reference model such as C-Model.[2,3] This is a large constructive solid geometry (CSG) MCNP model representing a 40-deg sector of the ITER device, with approximately 100 000 cells and surfaces, using universes to contain individual system models. The complexity of the model has resulted in the MCNP geometry creation and integration process becoming increasingly time-consuming and inefficient, often taking many months to simplify a system model and integrate it successfully into the reference C-Model geometry for analysis.

Ideally, one would be able to transition from a computer aided design (CAD) model to an identical radiation transport (RT) model ready for analysis, with no manual modification or repair of the resulting RT model. Design iterations could be performed on the CAD, and the RT model could be quickly updated and maintained in lockstep, which would enable a CAD-based design and optimization process to be applied to complex and realistic engineering models.

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The following issues have been found when implementing large complex universe–based models in MCNP, which prevent an efficient CAD-based modeling approach:

Issue 1: The need for significant CAD geometry simplification and manipulation to make it suitable for conversion to CSG (e.g., approximation of splines and splitting of bodies). This initial simplification can take many weeks; however, this does not prevent CAD iteration once simplified.

Issue 2: The need to repair converted MCNP models to remove interferences that lead to lost particles. These can occur even when the CAD is free of clashes. If edited by hand in the MCNP model, these changes would have to be performed for every reconversion.

Issue 3: The need to modify surfaces to avoid being coincident with the universe container cell. In MCNP, models containing surfaces coinciding with the universe sometimes lead to lost particles whose cause is particularly difficult to identify. Such modifications would need to be performed for every reconversion.

The solution to issue 1 is proposed to be the use of unstructured mesh geometry to reduce simplification requirements (e.g., tetrahedral volume mesh or faceted surface). Tolerance to very small overlaps and gaps (that often occur due to CAD numerical precision) in the RT code would address issue 2. Universe boundary errors in issue 3 are particularly problematic and require a universe implementation that is tolerant of coincident boundaries.

Serpent 2 (Ref. 4) has been investigated as a potential alternative to MCNP for ITER neutronics analysis. Other workflows may offer similar and/or alternative advantages and limitations, such as mesh-based MCNP6 or DAG-MCNP, the capabilities of which are discussed in a previous paper.[5] In this paper the features of Serpent 2 are discussed within the context of the three main issues affecting RT modeling. This paper also reports on some comparison of RT analysis results from Serpent and MCNP using an ITER-relevant model. Recommendations for future improvements are also discussed.

II. SERPENT 2 DEVELOPMENT STATUS AND FEATURES

The Serpent RT code, released in 2009, has established itself as a highly efficient program for nuclear reactor systems analysis. The current development version, Serpent 2, expands beyond reactor physics, and several capabilities have recently been developed that are applicable to ITER neutronics analysis. Serpent now supports coupled neutron-photon transport, which is essential for nuclear heating calculations; angular symmetry in universe fills (necessary to model a sector representation of ITER); and variance reduction capability in the form of weight windows (WWs) (required for efficient analysis of deeply shielded regions). It also has direct equivalents to most of the surface types contained in MCNP and supports universes, cell and mesh tallies, ENDF reaction rate tally multipliers (including heating), and custom response functions (e.g., flux–to–dose rate factors).

The physics routine currently implemented in Serpent 2 covers Rayleigh and Compton scattering, photoelectric effect, and electron-positron pair production for photon energies ranging from 1 keV to 100 MeV. Secondary photons are produced by atomic relaxation and bremsstrahlung, handled using the thick-target bremsstrahlung approximation. In addition to the standard ENDF cross-section libraries, Serpent 2 reads photon interaction data from supplementary data files. A more detailed description of the photon physics for Serpent can be found in Ref. 6.

Prior investigations have shown that unlike MCNP, Serpent does not suffer geometry errors when model surfaces are coincident with the universe boundary. Additionally, it supports tracking on unstructured volume meshes (like MCNP) and unstructured surface facets; this faceted CAD geometry approach is foreseen to be particularly useful for representing complicated components and reducing simplification requirements. The mesh-based geometry approaches also have tolerance to overlaps and support implicit background geometry (no need to model the void). The universe implementation in Serpent is highly general and supports models containing arbitrary numbers of CSG, mesh, and facet geometry in different universe fills in the same model. By supporting mixed geometry types, Serpent 2 has the potential to provide an easier routine to incorporate unstructured geometry into models that are currently MCNP based rather than CAD based, such as C-Model. The use of unstructured geometry types is beyond the scope of this paper; however, initial tests of stereolithography (STL) geometry against CSG have also been promising. Comparisons between STL geometry and CSG have been shown to yield equivalent results with little performance penalty.[5]

Given the above, Serpent 2 presents itself as a promising code for such analysis. Investigations have been undertaken in this work into the use of the Serpent 2 RT code for ITER neutronics analysis.

III. METHODOLOGY

A comparison between Serpent 2 and MCNP6 was performed to assess nuclear responses and computer requirements using the ITER C-Model. An automated conversion tool was developed using Python, which was able to rapidly create a Serpent 2 variant of the reference MCNP C-Model V1 R2.1 (Fig. 1) with equivalent cells and identical surface definitions. The ITER standard 14-MeV SDEF plasma source[7] was used in the MCNP C-Model. An equivalent source was created as a "C" routine for Serpent and verified. FENDL-2.1 (Ref. 8) neutron cross-section data were used in both cases. Photon cross-section data from the photon data library MCPLIB04/84 were used with MCNP and Serpent.

Analog calculations were performed both in MCNP6v1.0 and Serpent v2.1.29 to 10^9 histories, separately tallying the neutron and photon heating in each blanket, the divertor, the vacuum vessel, the toroidal field coils (TFCs), and the poloidal field coils (PFCs). Results for the neutron and photon flux spectra were also obtained in voxels of a mesh tally in the equatorial port plug (EPP) region. Results in deeper shielded components such as the PFCs were statistically poor, and a calculation was also attempted using variance reduction implemented through a global WW generated by ADVANTG (Ref. 9); unfortunately, issues were found with this feature of Serpent 2 and require further investigation.

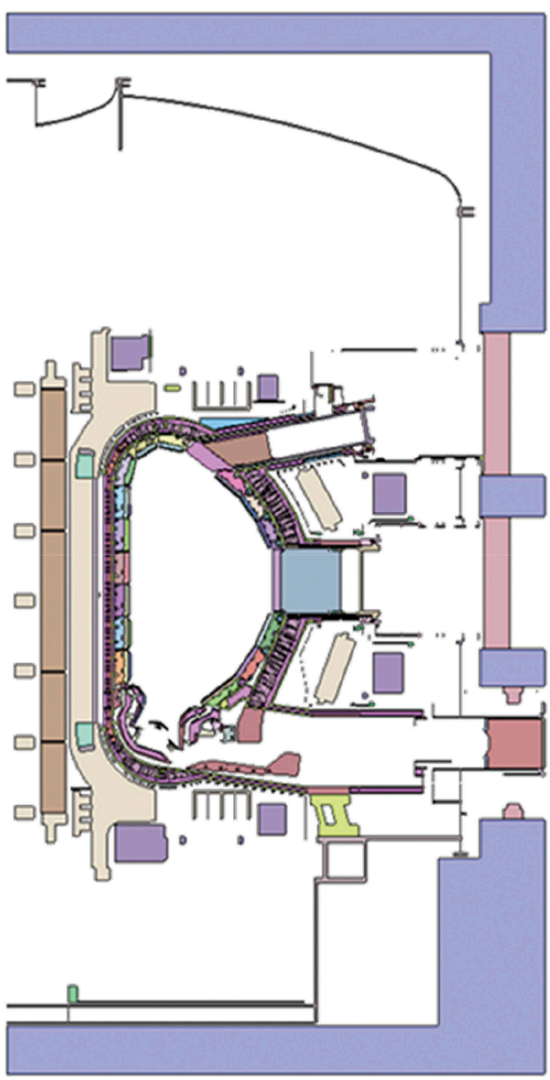


Fig. 1. ITER C-Model V1 R2.1 in Serpent 2.

IV. BENCHMARKING RESULTS

Calculations were run on an Intel Xeon E5-2665 cluster, with run times given in Table I. Results are plotted in Figs. 2 and 3 as the relative difference. Statistical errors were added in quadrature. Error bars on the plots are 1σ, based on the combined statistical error.

Results for neutron heating of blankets agreed within 0.4% of MCNP and for photon heating agreed within 0.3% across all blankets (Fig. 2). Neutron heating of the blankets in Serpent was noted to be slightly less than MCNP and outside statistics, though given that the comparison is between two different codes, the agreement is excellent. For the divertor, the neutron heating results were within 0.1% of MCNP, while the photon results were 1% higher. The reason for this was not clear, though again, the difference is small.

Except for some smaller components having high statistical error, the vacuum vessel neutron and photon heating results were within 0.5% of MCNP (Fig. 3). Heating tallies in the TFCs showed excellent agreement, while the PFC results had higher statistical errors and were difficult to compare.

The neutron and photon flux spectra were recorded in the 175-group (VITAMIN-J) structure in voxels of a

TABLE I

Basic Run Parameters

	MCNP 6	Serpent 2
Histories run	10^9	10^9
Cores	128	256 (32 MPI × 8 OMP)
Wall time (h)	19.7	31.9
Memory per MPI task (Gbyte)	2.9	37.6 (2.5 using opti 1[a])

[a]Opti 1 is an alternative optimization setting.

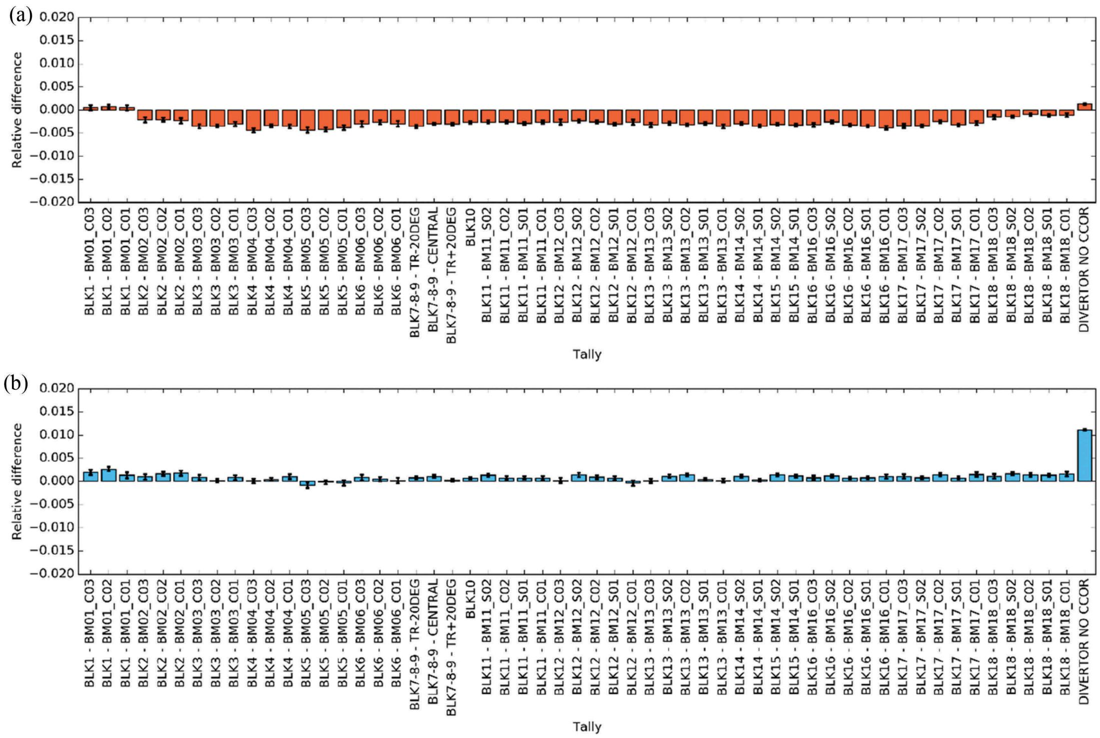


Fig. 2. Blanket and divertor heating results, difference relative to MCNP: (a) neutron and (b) photon.

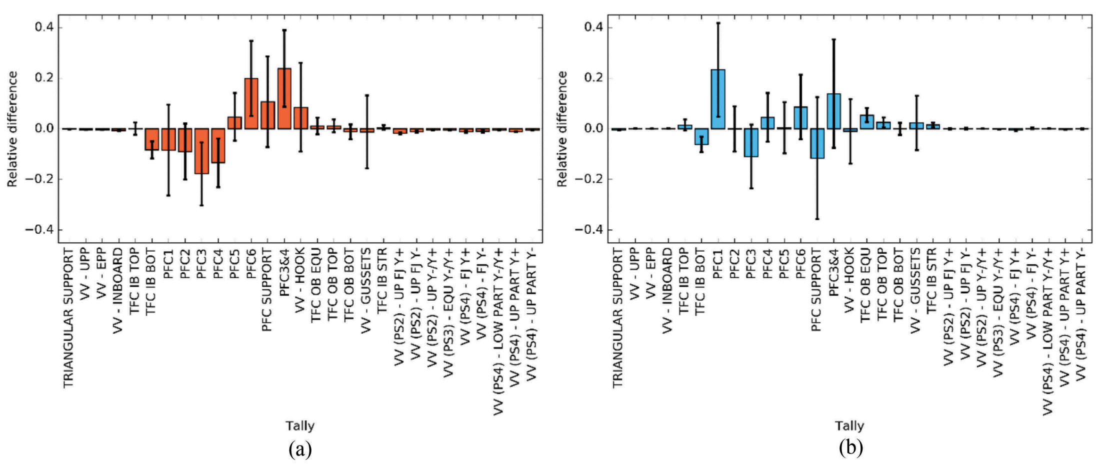


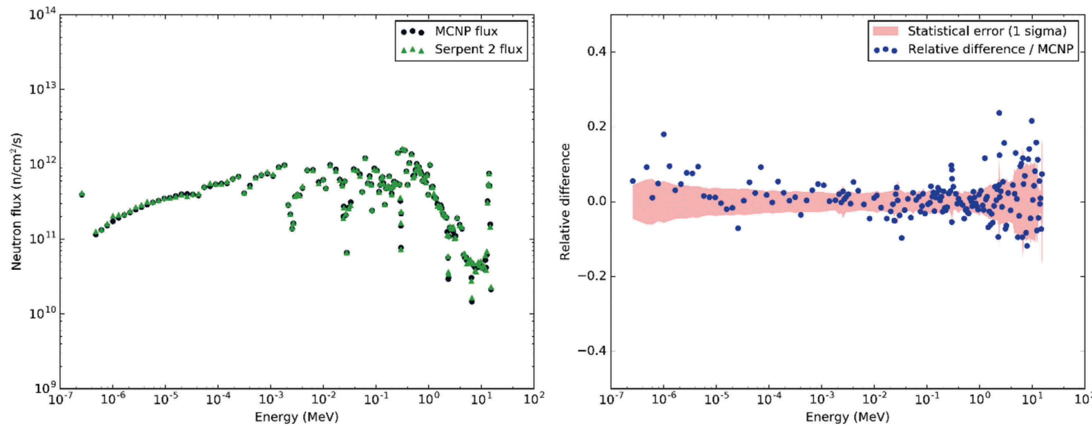
Fig. 3. Vacuum vessel and coil heating results, difference relative to MCNP: (a) neutron and (b) photon.

mesh tally in the EPP. The neutron spectrum is plotted against the bin midpoint for one voxel in the first-wall part of the EPP. Comparisons of the neutron and photon spectra in the front layer of the EPP showed excellent agreement within statistics (Figs. 4 and 5).

Comparisons were performed to assess the tally scoring efficiency for some of these results. The tally figure of merit (FOM) was analyzed accounting for the computer time T of the calculation and the resulting statistical error achieved R, as FOM = $1/R^2T$.

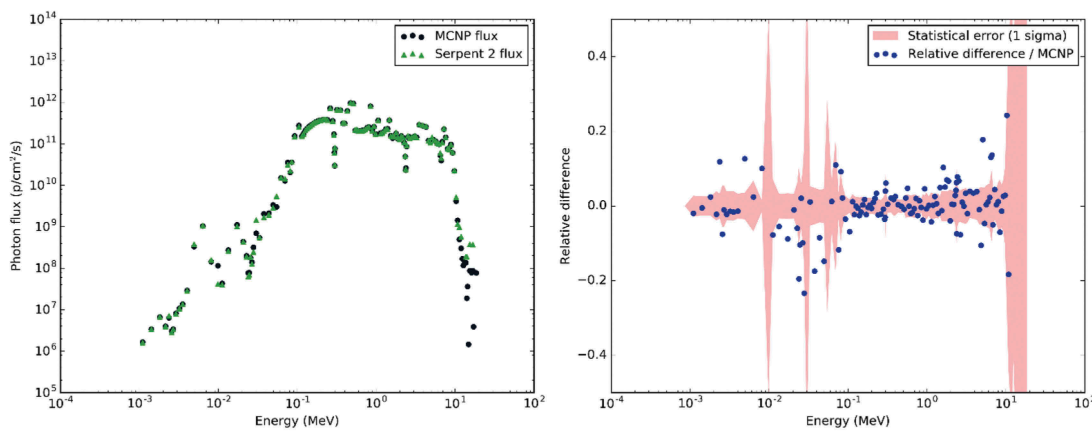
Across the blanket module tallies, the FOM for Serpent relative to MCNP was in the range 0.17 to 0.38. Tallies for the vacuum vessel and coils also fell within this range. As such, the tally FOM in Serpent was found to be typically three to five times lower than MCNP, thus requiring three to five times the computation time to achieve the same level of tally statistical accuracy.

The memory requirement per message passing interface (MPI) task for Serpent was initially found to be



(a) (b)

Fig. 4. Neutron flux spectrum in selected EPP mesh voxel: (a) flux and (b) difference relative to MCNP and error band.



(a) (b)

Fig. 5. Photon flux spectrum in selected EPP mesh voxel: (a) flux and (b) difference relative to MCNP and error band.

extremely high—almost 38 Gbytes per 8-threaded MPI task (this was broadly the same as a 1-thread task). There exists an optimization setting in Serpent to reduce memory use at the expense of computation time, and the default (mode 4, highest memory, fastest calculation) setting was used for the results presented here to maximize the speed of the Serpent calculations. Additional calculations were later performed using mode 1, and the memory usage dropped to 2.5 Gbytes per MPI task, while the FOM was reduced by only 3% and the results were within statistical uncertainty. Thus, in retrospect, for fusion neutronics calculations, mode 1 is recommended. Threaded [open multiprocessing (OMP)] parallelization was also found to be highly efficient in Serpent. With optimization mode 1, and using a hybrid MPI-OMP threading operation, Serpent has the potential to be highly memory efficient.

V. SUMMARY AND CONCLUSIONS

Comparisons have been undertaken between Serpent 2 and MCNP6 using a translated version of the C-Model V1 R2.1 model and ITER deuterium-tritium plasma source.

Results were compared for the blankets, divertor, vacuum vessel, TFCs, and PFCs within ITER standard tally cells. Coupled neutron-photon transport results for Serpent 2 were found to agree well with MCNP. Results showed some differences beyond computational statistics, though the agreement was still excellent, in general, and within 1% in many cases. Comparisons of neutron and photon spectra were also made in the first-wall layer of the EPP using a mesh tally, which again showed excellent agreement against MCNP.

These results clearly demonstrate that Serpent 2 generates results comparable to MCNP for ITER-relevant nuclear quantities in the ITER C-Model locations assessed.

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Comparisons of FOM were used to estimate the ability of the two codes to efficiently obtain a statistically reliable result. It was found that in the case of the analog calculation, Serpent 2 was typically between three and five times slower than MCNP 6 for the same model.

Memory use of Serpent was initially very high using the code defaults though was reduced to values comparable to MCNP in optimization mode 1, which is recommended for fusion neutronics applications as the performance penalty for this mode was found to be minimal.

Variance reduction in the form of WWs is a new feature in Serpent, which will be essential for performing most practical fusion neutronics and shielding analyses. The use of a WW was attempted in Serpent; however, this was not successful and requires further investigation.

While tally FOMs for Serpent 2 were typically a factor of 3 to 5 lower than MCNP, the code is at a beta stage of development, and future performance improvements may be possible. Furthermore, Serpent offers other benefits that have the potential to reduce the modeling time spent by the analyst, including support for surface mesh geometry representation and a universe implementation well-suited to the management of complex reference models that is tolerant of coincident boundary surfaces and offers support for mixed geometry types. Serpent 2 also supports hybrid (MPI-OMP) parallel acceleration, making efficient use of available machine memory.

Additional work is proceeding to compare Serpent 2 against experimental benchmarks relevant for fusion shielding problems to further demonstrate the suitability of Serpent 2 for ITER neutronics analysis as a complementary or alternative code to MCNP.

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