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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 modelling 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 D-T plasma neutron source was also created. Standard reference tallies in C-Model for the blanket and vacuum vessel heating were implemented and comparisons made between the two transport codes assessing nuclear responses and compute 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, compute requirements for Serpent were typically 3-5 times that of MCNP, and memory requirements broadly similar. Whilst slower than MCNP when applied to fusion neutronics, future developments may improve this, and the code offers clear benefits which will reduce analyst time, including: support for meshed geometry;

a robust universe implementation which 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. Whilst 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.

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]. This is a large constructive solid geometry (CSG) MCNP model representing a 40° 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 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 quickly updated and maintained in lock-step, which would enable a CAD-based design and optimisation process to be applied to complex and realistic engineering models.

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

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.

2. The need to repair converted MCNP models to remove interferences which 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 re-conversion.

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 re-conversion.

The solution to (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 overlaps and gaps in the RT code would address (2). Universe boundary errors (3) are particularly problematic and require a universe implementation that is tolerant of coincident boundaries.

Serpent 2 (Ref. 3) has been investigated as a potential alternative to MCNP for ITER neutronics analysis. This paper reports on some testing of Serpent against MCNP using an ITER-relevant model. Comparisons between the codes are discussed and recommendations made for future improvements.

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 (required for efficient analysis of deeply shielded regions). It also has direct equivalents to most of the surface types contained in MCNP, supports universes, cell and mesh tallies, ENDF reaction rate tally multipliers (including heating) and custom response functions (e.g. flux to dose rate factors).

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 which are currently MCNP 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 STL geometry against CSG have also been promising; comparisons between STL and CSG geometry have been shown to yield equivalent results with little performance penalty[4].

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 radiation transport code for ITER neutronics analysis.

III. Methodology

A comparison between Serpent 2 and MCNP6 was performed to assess nuclear responses and compute 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 rev. 2.1 (Fig.1) with equivalent cells and identical surface definitions. The ITER standard 14 MeV 'SDEF' plasma source[5] was used in the MCNP C-Model. An equivalent source was created as a 'C' routine for Serpent and verified. FENDL-2.1 (Ref. 6) neutron cross-section data was used in both cases.

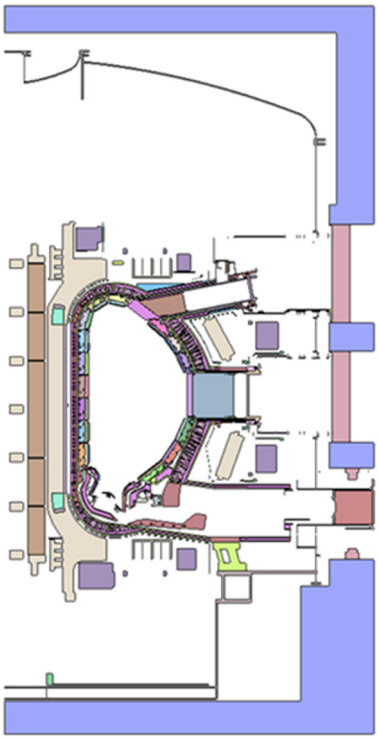

Fig. 1. ITER C-Model rev. 2.1 in Serpent 2

Analogue 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, vacuum vessel, toroidal field coils (TFC) and poloidal field coils (PFC). Results for the neutron and photon flux spectra were also obtained in voxels of a mesh tally in the equatorial port plug region. Results in deeper shielded components such as the PFC were statistically poor, and a calculation was also attempted using a global weight window generated by ADVANTG[7]; unfortunately, issues were found with this feature of Serpent 2 and requires further investigation before a fuller comparison can be made.

IV. Benchmarking results

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

Table I. Basic run parameters.

	MCNP 6	**Serpent 2**
Histories run	10^9	10^9
Cores	128	256 (32 MPI x 8 OMP)
Wall time (h)	19.7	31.9
Memory (GB) per MPI task	2.9	37.6 (2.5 using 'opti 1')

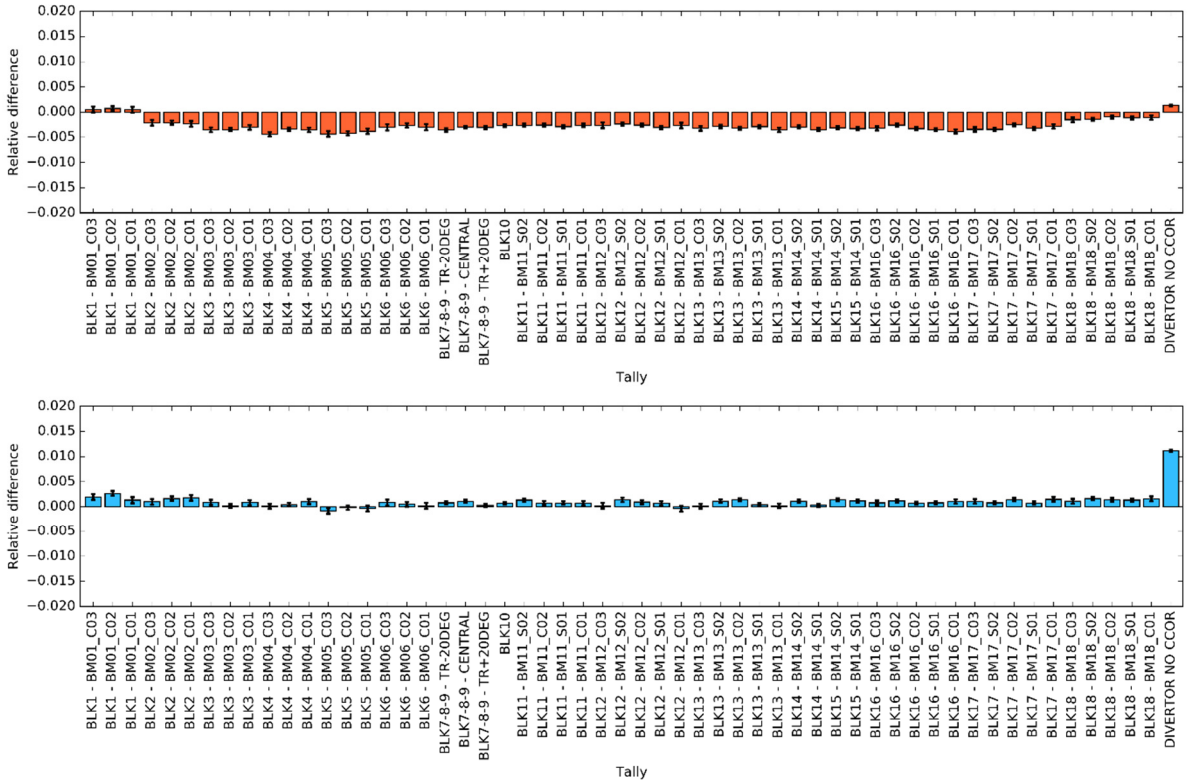

Fig. 2. Blanket and divertor heating results, difference relative to MCNP (top: neutron, bottom: photon)

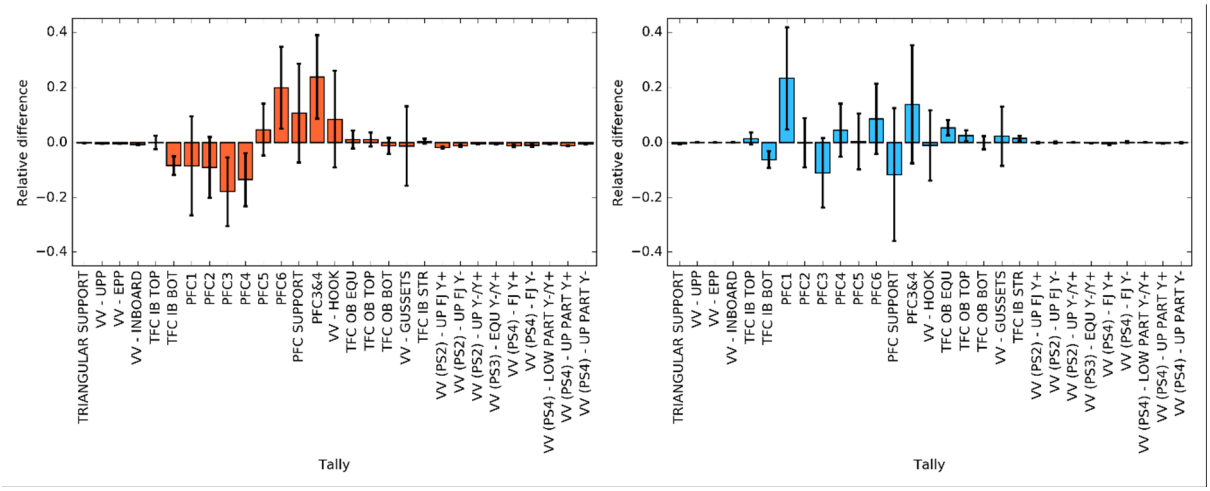

Fig 3. Vacuum vessel and coils heating results, difference relative to MCNP (left: neutron, right: photon).

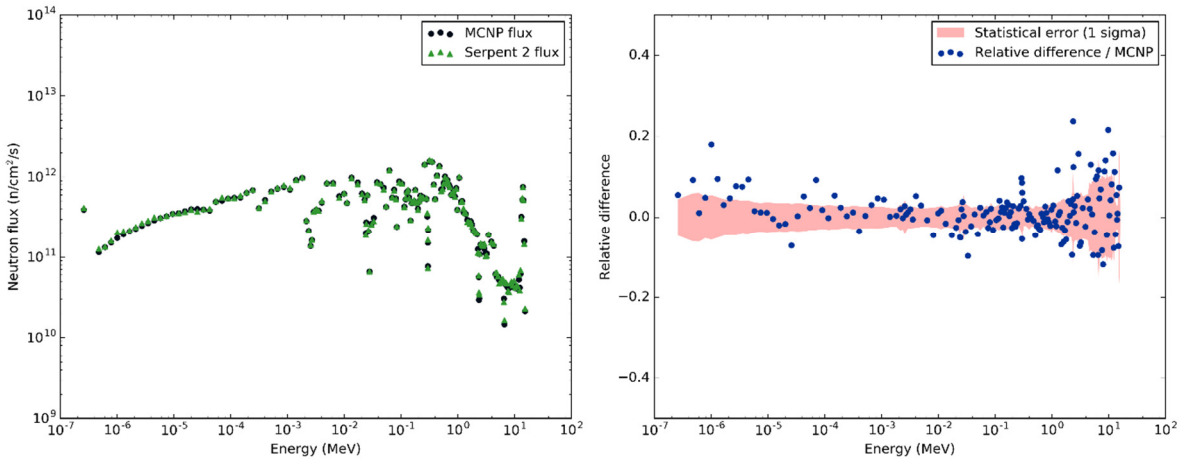

Fig 4. Neutron flux spectrum in selected EPP mesh voxel (left: flux, right: difference relative to MCNP and error band)

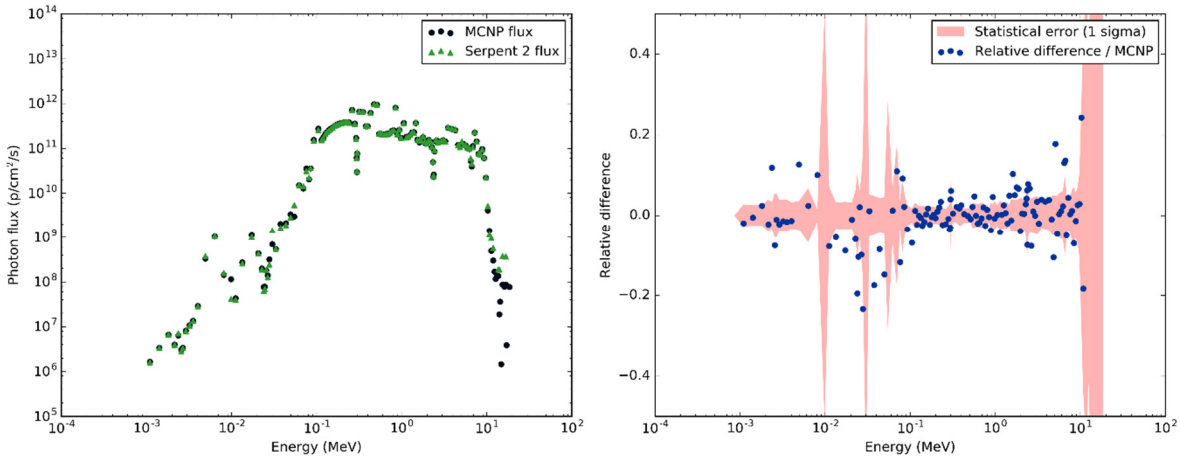

Fig 5. Photon flux spectrum in selected EPP mesh voxel (left: flux, right: difference to MCNP and error band)

Results for neutron heating of blankets agreed within 0.4% of MCNP, and for photon heating, 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 the comparison is between two different codes, the agreement is excellent. For the divertor, neutron heating results were within 0.1% of MCNP, whilst 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 TFC showed excellent agreement, whilst 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 mesh tally in the equatorial port plug (EPP). The neutron spectrum is plotted against 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 (Fig 4, Fig 5).

Comparisons were performed to assess the tally scoring efficiency for some of these results. The tally figure of merit (FoM) was analysed accounting for the compute 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 – 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 3 to 5 times lower than MCNP, thus requiring 3-5 times the compute to achieve the same level of tally statistical accuracy.

The memory requirement per MPI task for Serpent was initially found to be extremely high – almost 38 GB per 8 threaded MPI task (this was broadly the same as a 1-thread task). There exists an optimisation setting in Serpent to reduce memory use at the expense of

compute time, and the default (‘mode 4’, highest memory, fastest calculation) setting was used for the results presented here to maximise the speed of the Serpent calculations. Additional calculations were later performed using ‘mode 1’ and the memory usage dropped to 2.5 GB per MPI task, whilst the FoM only reduced by 3%. Thus, in retrospect, for fusion neutronics calculations ‘mode 1’ is recommended. Threaded (OMP) parallelisation was also found to be highly efficient in Serpent. With optimisation mode 1, and using 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 rev. 2.1 model and ITER DT plasma source.

Results were compared for the blankets, divertor, vacuum vessel, TFC and PFC 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 in general excellent, 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.

Comparisons of figure of merit (FoM) were used to estimate the ability of the two codes to efficiently obtain a statistically reliable result. It was found in the case of the analogue calculation, that Serpent 2 was typically between 3-5 x slower then 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 ‘mode 1’ optimisation, which is recommended for

fusion neutronics applications as the performance penalty for ‘mode 1’ was found to be minimal.

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

Whilst tally figures of merit for Serpent 2 were typically a factor of 3-5 lower than MCNP, the code is at a beta stage of development and future performance improvements may be possible. Furthermore, Serpent offers other benefits which have the potential to reduce the modelling time spent by the analyst, including: support for surface mesh geometry representation; a universe implementation well-suited to the management of complex reference models, which is tolerant of coincident boundary surfaces, and offers support for mixed geometry types. Hybrid (MPI-OMP) parallel acceleration makes efficient use of available machine memory, and license conditions permitting the use of national computing facilities.

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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