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Optimising differential data formats for Monte-Carlo radiation transport in the fusion regime

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ABSTRACT

Monte-Carlo based radiation transport codes are widely used to simulate the behaviour of nuclear facilities, to aid their design, operation and inform on safety aspects. The accuracy, and hence reliability, of the output of transport codes is entirely dependent on the underlying nuclear data. The formalism used in the processed data directly impacts on the computational performance for such calculations. For example, low data density results in faster computation possibly made at the expense of accuracy and vice versa. A current standard transport code, MCNP, requires pre-processing and reformatting of raw nuclear data files (ENDF) before their use within the simulation. The incident particles angular distribution is usually processed to an equal probability histogram with 32 channels, or to a set of data points with linear interpolation across the angular and energy range. The former method is fast to sample, yet sacrifices the accuracy of the data representation. The latter method provides a better representation of the original format, but has a tendency to produce larger data files that are correspondingly slower to sample. This study considers the relative accuracies of these processing formalisms and the relationship to computational efficiency via an in-house, simplified Monte-Carlo code. For future code developments within the fusion community, we consider variations upon both methods in an effort to determine the optimal balance between computational efficiency and accurate data representation. We also attempt to quantify the effects of a lesser accuracy versus high computational burden in the simulation of fusion reactor design.

1. Introduction

Nuclear data underpin many aspects of nuclear science and technology; this work focuses on the relevance of nuclear data to fusion reactor design. Nuclear data refer to the parameters that describe the underlying physics of an engineering relevant problem. In the case of fusion neutronics, neutron interaction cross-section data are used within radiation transport codes to determine global parameters such as shut-down dose rates, tritium breeding ratios or shielding requirements. The reliability of these global parameters is directly related to the quality of the output, i.e. garbage in, garbage out. For fusion applications we require a full complement of materials data, with a high importance placed on differential data. This data determines the angular and energy behaviour of radiation quanta. Areas within the fusion domain that are most reliant on accurate data include tritium breeding (Soltani et al., 2015), activation (Sheludjakov and Serikov, 2002) and shielding analyses (Fausser et al., 2011). Nuclear data for fusion applications is lacking in many areas due to the difficulty of measuring the required quantities; the level of confidence in simulation results is limited by the availability and quality of this experimental data. Future plans to develop and construct commercially viable fusion reactors are entirely reliant on the ability to predict and minimise the engineering tolerances. This can only be achieved by determining where inaccuracies occur within the data, quantify them, and finally minimise them.

From experimental measurement through to use in radiation transport simulations, a lengthy and complicated process is undertaken, as demonstrated by the nuclear data cycle in Fig. 1. By better understanding the nature and behaviour of data errors during the cycle, we can attempt to quantify their effect on design tolerances, and once highlighted, efforts can be taken to minimise them. Examples of propagation of experimental and evaluation uncertainties can be found in García-Herranz et al. (2008) and Rochman et al. (2011) and the importance of uncertainty propagation is gaining recognition within the fusion community. These studies, among others, have demonstrated a sensitivity of radiation transport simulations to small perturbations in the nuclear data.

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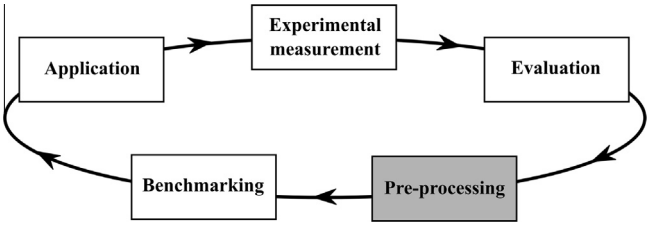

Fig. 1. The nuclear data cycle starts with experimental measurements of differential and integral quantities, and are uploaded to the EXFOR database (Otuka et al., 2014). These measurements are discrete, yet data in radiation transport codes must be continuous, so evaluators pick relevant data points from experiment and fill in the gaps using nuclear model codes. Data is output into general purpose ENDF (Evaluated Nuclear Data Format) files (Chadwick et al., 2011) and built into libraries. Due to the wide range of uses in various codes these libraries must be processed into code specific formats. In this work we consider the processing to ACE (A Compact ENDF) for use in MCNP. Any new data and libraries must be benchmarked against experimental data to validate the physicality of data before it can be trusted for use in nuclear facility design. The intended end use determines the future experimental requirements.

We extend this to determine the effect of pre-processing on the accuracy of data within the context of the nuclear data cycle shown in Fig. 1. Pre-processing methods were designed for legacy applications, and the methods have not significantly changed since. For legacy applications, pre-processing was considered to have a negligible impact upon data fidelity. When applied to non-legacy data, such as for fusion, pre-processing can compromise the accuracy and hence critical information may be lost (Hutton et al., 2015). Fusion systems tend towards fixed source, shielding penetration simulation problems compared to fission systems where the neutron map tends to be evenly distributed within a core made of an ensemble of regular pin-cell assemblies.

The transport of neutrons can be mathematically approximated by neutron transport equation, as shown in Eq. (1) (Duderstadt, 1976). This equation covers a seven dimensional phase space, three in space ($\vec{r}$), two in angle ($\vec{\Omega}$) and one in energy (E) and time (t); where ϕ is the angular flux density and is a function of $\vec{r}, E, \vec{\Omega}$ and t. It is too computationally intensive to solve the full transport equation, there are methods of discretising the phase space to simplify the problem, but these result in the loss of physical representation. The Monte-Carlo method is an alternative to solving the transport equation; instead we directly simulate large numbers of neutrons and rely on the stochastic nature of their interactions with matter. From these simulations we can infer the average behaviour of neutrons within the system, based on the central limit theorem. The nature of the interactions are determined by random sampling of the cross section data, Σ (the probability for a certain interaction to occur) and are contained within data libraries.

$$\frac{1}{v}\frac{\partial}{\partial t}\phi + \nabla.\vec{\Omega}\phi + \Sigma_{total}(E)\phi = \int_0^{4\pi}\int_0^{\infty}\Sigma_{scatter}(E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega})\phi dE' d\vec{\Omega}' + S \quad (1)$$

The evaluated data files contain vast amount of interaction data, and the nature of data pre-processing varies from one section to another. The interaction cross sections are evaluated on a fine energy grid to include resonances and the differential cross sections (exit angle and/or energy of radiation quanta post interaction) are discretised to improve sampling efficiency, at the cost of data fidelity. The differential data contributes 60%, on average, to the file content. Functional sets of data can be processed into one of two distinct formats; equal probability histograms, or linearly interpolated, tabulated probabilities. We focus on the formats used by the radiation transport code MCNP (Monte-Carlo N-Particle) (Briesmeister, 1993). This code accepts ACE (A Compact ENDF) formatted files only, processed with NJOY (MacFarlane et al., 2013). The standard outputs is a fixed 32 equal probability bin method; this has a small data overhead and is very fast to sample across all channels, but this compromises on the accuracy of data replication for high energy applications (Hutton et al., 2015). More recently data libraries have been processed into the tabulated cumulative law format and this is considered to provide a more accurate depiction of the original data at the cost of increased sampling time and memory requirements. This work considers the accuracy of different data processing formalisms and their relationship to computational burden when compared to the current default methods. In particular we look at their use in fusion reactor simulations, such as the ITER (International Thermonuclear Experimental Reactor). The MCNP model for this device is shown in Fig. 2. For a typical run we require 10^{12} neutron histories to fully populate the model throughout the volume, which corresponds to 9.4 days of computational runtime and 866 MB of physical memory to store the interaction data (Davis and Turner, 2011). The Monte Carlo method is computationally intensive by nature and the model in Fig. 2 is a simplified version of the full device.

2. Approach

The differential components of the evaluated data files (ENDF) span the full energy and angular ranges of the different interactions; two excerpts from the files are shown in Fig. 3. This shows

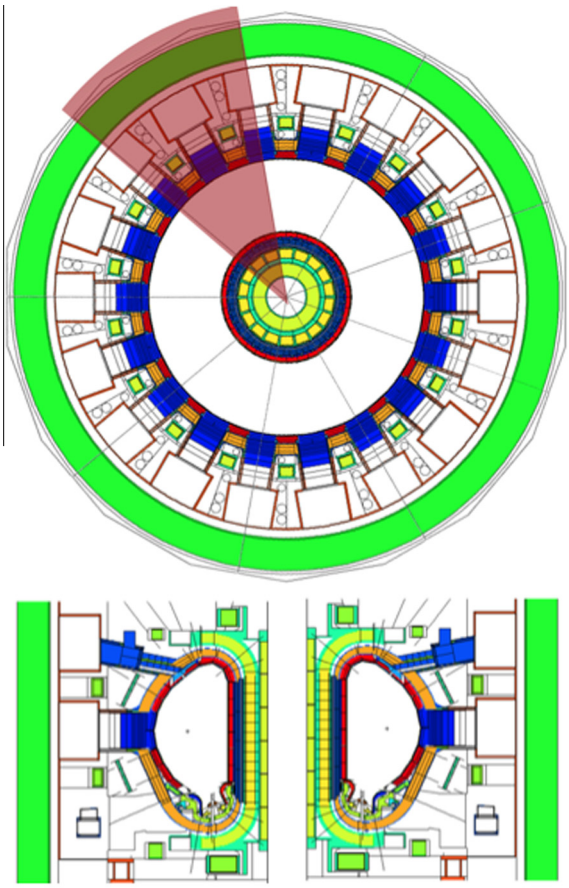

Fig. 2. MCNP model of the ITER tokamak (Loughlin et al., 2009), due to the need for computational efficiency, the symmetry of the system is utilised and only a 40° segment is simulated (highlighted). The model contains 8500 cells filled with 212 different materials, created from 63 different isotopes, with dimensions of around 2 m radially and 2.5 m in height. If we make the model more physical, both in geometry and data terms, we increase the computational burden and the complexity and resolution of the data files.