Neutronics and Nuclear Data for Fusion Technology - Recent Achievements in the EU Programme

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Abstract. An overview is presented of the progress achieved in the EU over the past two years in the field of neutronics and nuclear data for fusion technology. Significant progress has been achieved in making available new data evaluations for neutron transport and activation calculations satisfying the needs for applications to ITER, the International Thermonuclear Experimental Reactor, and the intense neutron source IFMIF ("International Fusion Material Irradiation Facility"), in developing advanced computational tools such as the CAD interface programme for the MCNP code, in extending the capabilities for Monte Carlo based calculations of sensitivities & uncertainties by using the track length estimator, and, in providing the experimental data for a breeder blanket mock-up required for validating related neutronics design calculations.

1. Introduction

The nuclear design of any kind of fusion device relies upon the results of neutronics calculations. Neutronics and nuclear data thus play a key role in the strategic approach to develop fusion as a future energy source. A well-qualified nuclear database and validated computational tools are required for quality assured neutronics and activation calculations including uncertainty assessments. In the framework of the European Fusion Technology Programme, the efforts focus accordingly on the development and qualification of computational tools and data required for reliable design analyses of ITER, the International Thermonuclear Experimental Reactor [1], in particular the layout of the Test Blanket Modules (TBM), and the intense neutron source IFMIF ("International Fusion Material Irradiation Facility") [2]. A major effort is devoted to integral experiments with the objective to provide the experimental data base for testing the nuclear data and validating neutronics design calculations.

The objective of this paper is to present the progress achieved in the EU over the past two years in the field of neutronics and nuclear data for fusion technology. Significant progress has been achieved in (1) making available new data evaluations for neutron transport and activation calculations satisfying the needs for both ITER and IFMIF applications, in (2) developing advanced computational tools such as the CAD interface programme for the MCNP code, and (3) in extending the capabilities for Monte Carlo based calculations of sensitivities & uncertainties by using the track length estimator, and, (4) in providing the experimental data for a breeder blanket mock-up required for validating related neutronics design calculations. In the following an overview of the recent achievements in the respective fields is presented.

2. Nuclear data evaluations and libraries for fusion technology

With the European Fusion File (EFF) and the European Activation File (EAF) projects the EU is conducting a unique effort on the development of nuclear data libraries dedicated to fusion technology (FT) applications [3]. The EFF data evaluations are integrated into the Joint Evaluated Fission and Fusion File (JEFF) [4] which represents a complete data library of general purpose data evaluations satisfying both fission and fusion needs.

The recent EFF evaluation effort was devoted to the reaction systems n + $^{182, 183, 184, 186}$W [5] and n + ^{181}Ta [6] covering the energy range up to 150 MeV. Use was made of the nuclear model codes ECIS96 [7] for optical model calculations and GNASH [8] for nuclear reaction cross section calculations including the pre-equilibrium emission of multiple particles. High energy experimental data were taken into account in evaluating the total cross section whenever available. Global optical model potentials were used for neutrons, protons, deuterons and α-particles. Optical model potentials for tritons and He-3 were constructed on the basis of proton and neutron potentials. To improve the neutron emission spectra, collective excitations were included in the GNASH calculations. Double-differential cross sections of the emitted particles were calculated on the basis of the Kalbach systematics. The general purpose data files were prepared in standard ENDF6 data format and processed with the NJOY code [9] for Monte Carlo transport calculations with MCNP [10]. The ENDF data files are currently being complemented by co-variance data. The new evaluations are in good agreement with measured cross section data as shown in Figs. 1a,b for the examples of the ^{181}Ta(n,xn) neutron emission spectra at 14 and 20 MeV incident neutron energy.

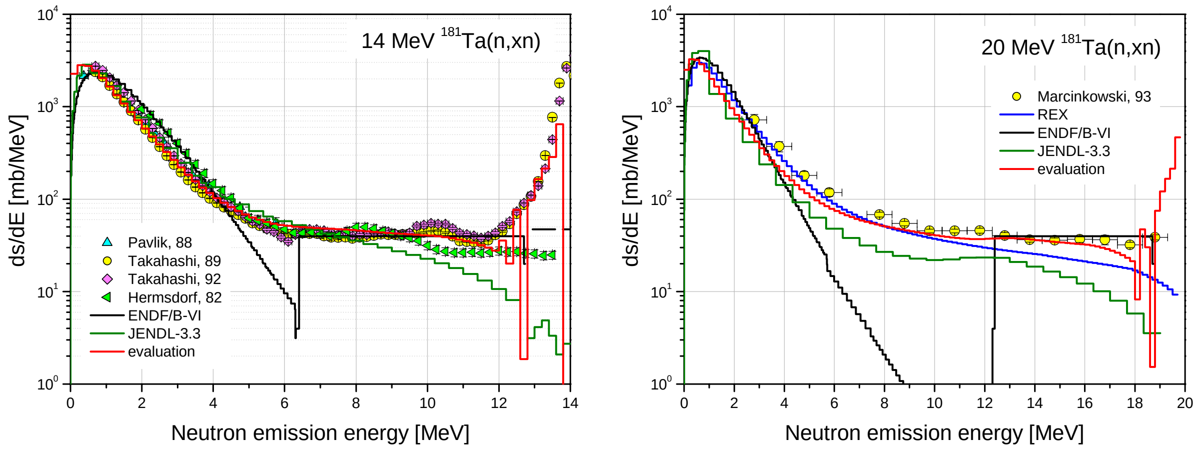

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FIG. 1a : 14 MeV incident neutron energy *FIG. 1b: 20 MeV incident neutron energy*

FIG . 1 a,b: Evaluated and measured neutron emission spectra for the reaction system n + ^{181}Ta.

To provide the data for describing the neutron source generation in the Lithium target of the IFMIF neutron source by means of the McDeLicious Monte Carlo code [11], a complete new evaluation of the d + ^{6,7}Li interaction cross sections up to 50 MeV deuteron energy has been performed. A new methodology was applied which takes into account compound nucleus reactions, pre-equilibrium processes, stripping and direct interactions [12]. Fig. 2 shows, as an example, the calculated double-differential neutron emission cross section and its breakdown into the different reaction components for 40 MeV incident deuterons. It is revealed that the inclusion of direct interaction processes is essential for representing the structures of the emission cross section at high neutron energies. This is due to the fact that the direct reaction mechanism is dominant for the emission of neutrons with energies above the deuteron incidence energy.

A series of benchmark calculations was performed with the McDeLicious code to test the new data against experimental thick Lithium target neutron yields. The comparison of measured and calculated forward neutron yields, Fig. 3, shows that McDeLicious with the updated d-Li cross section data is well able to reproduce the experimental results over the entire deuteron energy range from threshold up to 40 MeV. The approaches of McDeLi [13], the predecessor to McDeLicious, and the MCNPX code [14] using the ISABEL intra-nuclear cascade model, give significant worse agreement with the experimental neutron yields.

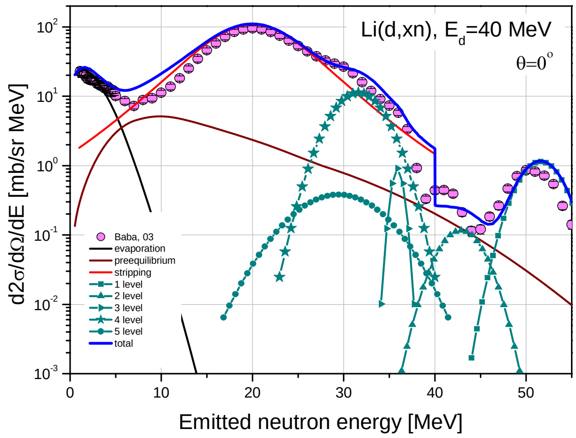

FIG. 2: Measured and evaluated ^{7}Li(d,xn) double differential neutron emission cross section for 40 MeV incident deuteron energy.

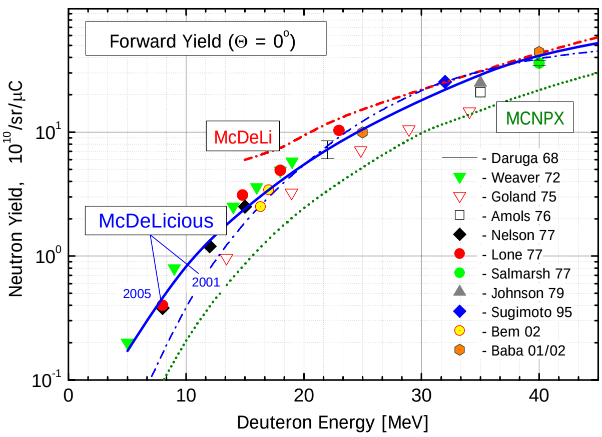

FIG. 3: Measured and calculated thick lithium target forward neutron yield as function of the deuteron energy.

The comparison of McDeLicious calculations for neutron angular differential yields using the new d-Li evaluation showed that the angular dependence can be satisfactorily predicted over the whole range of measured deuteron energies and secondary neutron angles [12]. The other two approaches show again a worse reproduction of the experimental data set, especially below 20 MeV. The comparison of McDeLicious calculations with measured double-differential thick target neutron yields demonstrates also significant improvements with the updated d-Li evaluation. Thus a clear improvement of the prediction accuracy was obtained for the IFMIF neutron source term simulation with McDeLicious employing the new d + ^{6,7}Li cross section data evaluations.

A major evaluation effort has been conducted on the production of a qualified activation data library for fusion inventory calculations. This has led to various versions of the European Activation File (EAF) with the current version EAF-2005 with an extended energy range up to 60 MeV [15]. The EAF-2005 activation file thus satisfies the needs for activation calculations of the IFMIF neutron source and contains cross section data of 62,637 neutron-induced reactions. Using available integral data, the library has been extensively validated both for the energy range below and above 20 MeV [16,17]. A first version of a deuteron-induced activation data library has been generated in early 2006 to enable the assessment of the activation of IFMIF accelerator components by deuteron beam losses [18]. This preliminary library is entirely based on model calculations with the TALYS code [19] using global parameters. The library is currently being updated using improved model calculations and available experimental data. This new library will form part of EAF-2007 planned for release next year.

3. CAD geometry data for Monte Carlo calculations

The Monte Carlo technique enables the use of full and detailed 3D geometry models in neutronics calculations. The manual modelling of a complex geometry with a Monte Carlo code, as it is common practice, is an extensive, time-consuming and error-prone task. A more efficient way is to make use of available CAD geometry data in the Monte Carlo calculations. This can be achieved by converting the CAD data into the semi-algebraic representation used by Monte Carlo codes such as MCNP. Suitable conversion algorithms have been previously developed [20] and have been implemented into an interface programme with a graphical user interface (GUI) called McCAD [21].

The McCAD interface programme integrates a CAD kernel, a C++ GUI application framework, and the conversion algorithm. The CAD kernel provides core data structures, algorithms, and data exchange interfaces for neutral CAD data files such as IGES and STEP. The GUI framework provides data structures for visualization and user operations. McCad is also capable of generating a CAD geometry model from an MCNP input deck.

The typical McCAD processing flow is as follows. A geometry model, suitable for neutron transport calculations, is generated with a CAD system. The suitability is determined by the inherent limitations of MCNP with regard to the geometry representation and the adequacy of the model for the neutron transport with regard to complexity. In particular, the CAD geometry model must be constructed in the boundary representation (B-rep) with algebraic boundary supports such as planes, quadrics and tori, and no free-form surfaces. The only limitation from the algorithmic point of view is that the model should represent a manifold solid, or a collection or an assembly of solids, described in a B-rep data structure. The CAD model is transferred to the interface via data files in the IGES (version 5.3) or STEP neutral format. Both file formats are able to transform B-rep data structures accurately. McCAD then performs automatically model suitability and error checks, and, if possible, repairs. Suitability checks are limited to geometric properties, i.e., the check if the boundary supports are algebraic. Geometrical and topological errors are checked for gaps and overlaps between boundary entities as well as small boundary entities. The next step is then the conversion of the data which is followed by checks for overlaps among solids and their repair. Finally, the model is completed by voids and output in the standard MCNP syntax. This file can be used directly by MCNP after completion with other required data such as materials specifications, cross section data, source definition, and tally specifications etc.

Successful test applications have been previously performed for an octant of JET [22] and recently for a 40 degree torus sector of ITER [23] demonstrating the capability for the automated processing of the CAD data and their conversion into a geometry model for Monte Carlo calculations with the MCNP code. Current design applications include the generation and use of MCNP models for the Electron Cyclotron Resonance Heating (ECRH) in the upper port of ITER.

As an example, Fig. 4a shows the CAD model of the 40 degree ITER torus sector consisting of all components relevant for the neutronic analyses. Starting from a CAD geometry model provided by the ITER International Team, Garching, this model was elaborated at FZK with the CATIA V5 software following the guidelines for the generation of CAD neutronics models. The converted MCNP model, generated automatically by McCAD, is shown in Fig. 4b in a vertical cut as provided by the MCNP geometry plotter. It is noted that the conversion process does not introduce any approximations.

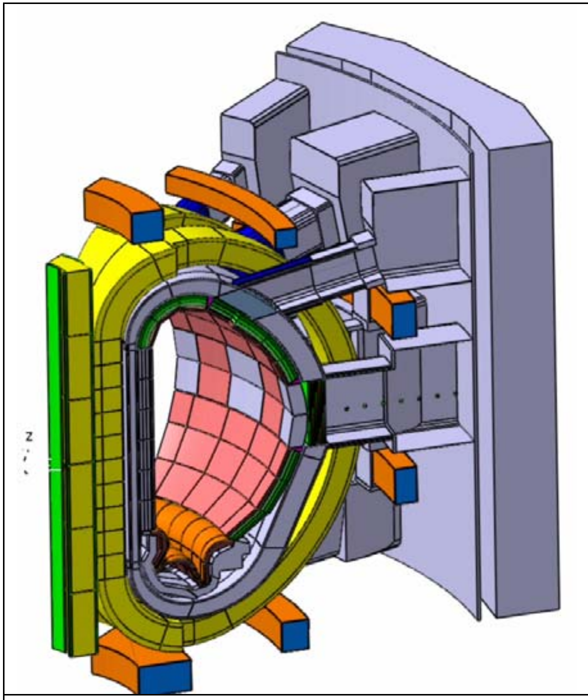

FIG 4a: CAD model of ITER 40 ° torus sector (CATIA V5)

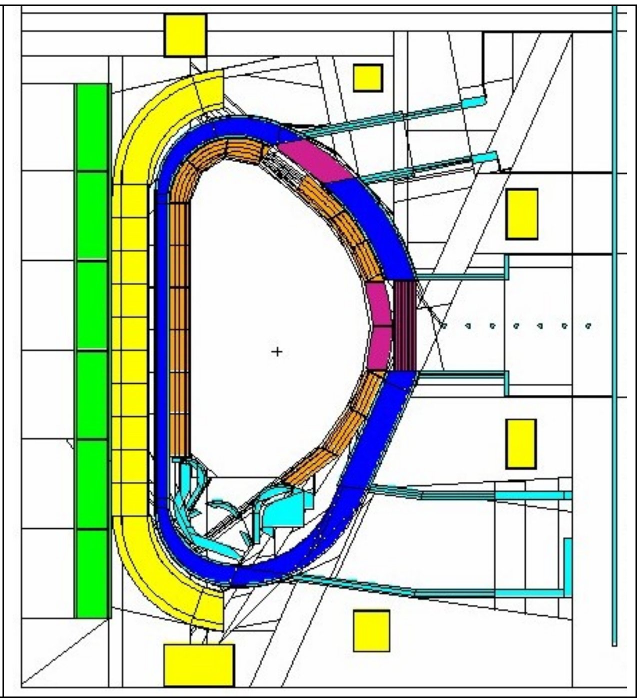

FIG. 4b: Converted MCNP model (2D radial-poloidal cut by MCNP plotter)

FIG. 4 a, b: Comparison of CAD and MCNP models converted by the McCAD interface

The converted geometry was first checked by means of volume comparison calculations for the CAD and the converted models. The volumes of the CAD model could be well reproduced by stochastic MCNP volume calculations using the converted model thus confirming the proper working of the conversion process. A series of transport calculations was next performed starting with the calculation of the neutron wall loading distribution. Further validation calculations including neutron flux and nuclear heating calculations are currently underway in the frame work of a related ITER benchmark exercise.

4. Monte Carlo based sensitivity/uncertainty calculations

Sensitivity and uncertainty analysis is a powerful means to assess uncertainties of nuclear responses in neutron transport calculations and track down them to specific nuclides, reaction cross-sections and energy ranges. A method to calculate sensitivities of Monte Carlo point detector responses has been previously developed [24] and implemented in a local version of MCNP4c, called MCSEN. This method has been extended to include sensitivities to secondaries' angular distributions (SAD) [25].

The Monte Carlo based calculation of uncertainties of nuclear responses in the Test Blanket Modules (TBM) of ITER requires the capability to calculate sensitivities for responses by the track length estimator. Suitable algorithms based on the differential operator method were developed to this end and implemented in MCSEN code. This enables the efficient calculation of sensitivities for neutron fluxes and nuclear responses such as reaction rates in a geometry cell of an arbitrary 3D geometry. Sensitivities can be calculated to reaction cross sections, the material density and secondaries' angular distributions. Verification tests were performed by comparing the sensitivities calculated with the track length estimator in a cell and sensitivities calculated by the point detector.

In a first real application, a sensitivity/uncertainty analysis was performed for the neutronics experiment on a mock-up of the HCPB (Helium-Cooled Pebble Bed) TBM employing the track length estimator feature of MCSEN [26]. The dominant tritium production from ^{6}Li, e. g. was shown to be mainly sensitive to the Be cross-sections for the elastic scattering (1.7 – 2.1 %/%) and the (n,2n) reaction (0.7 %/%). The uncertainties of the total Tritium Production Rate (TPR) due to uncertainties of the reaction cross-sections are at 4% (2σ confidence level) and are dominated by the ^{9}Be uncertainties. The total TPR uncertainties including the data uncertainties, the statistical uncertainties of the Monte Carlo calculation and the experimental uncertainties are in the order of 8 to 10 % (2σ), see Table 1.

TABLE 1: TOTAL UNCERTAINTIES (2σ) OF THE TPR IN THE HCPB TBM MOCK-UP

	Stack 1	Stack 3	Stack 5	Stack 7
Calculation				
MC calculations	2.6%	2.8%	3.3%	4.2%
Data uncertainty	3.5%	4.3%	4.0%	3.5%
Calculation + data uncertainty	4.4%	5.2%	5.2%	5.5%
Experiment				
Neutron source uncertainty	6.0%	6.0%	6.0%	6.0%
Measurement uncertainty	3.2%	5.1%	4.8%	5.2%
Total uncertainty (exp. + calc. + data)	**8.1%**	**9.4%**	**9.3%**	**9.6%**

5. Neutronics breeder blanket benchmark experiment

The current focus of the experimental benchmark effort in the EU is on neutronics TBM mock-ups. A first experiment has been performed at the Frascati Neutron Generator (FNG) on a TBM mock-up of the HCPB breeder blanket to check and validate the capability of the neutronic codes and nuclear data to predict its Tritium Production capability [27]. The mock-up replicates the main characteristics of a breeder insert of the TBM HCPB in ITER. It consists of a stainless steel box with outer dimensions of 31x31x29 cm, filled by alternating layers of breeder material (Li_2CO_3) and neutron multiplier (Be), see Fig. 6 for the MCNP model.

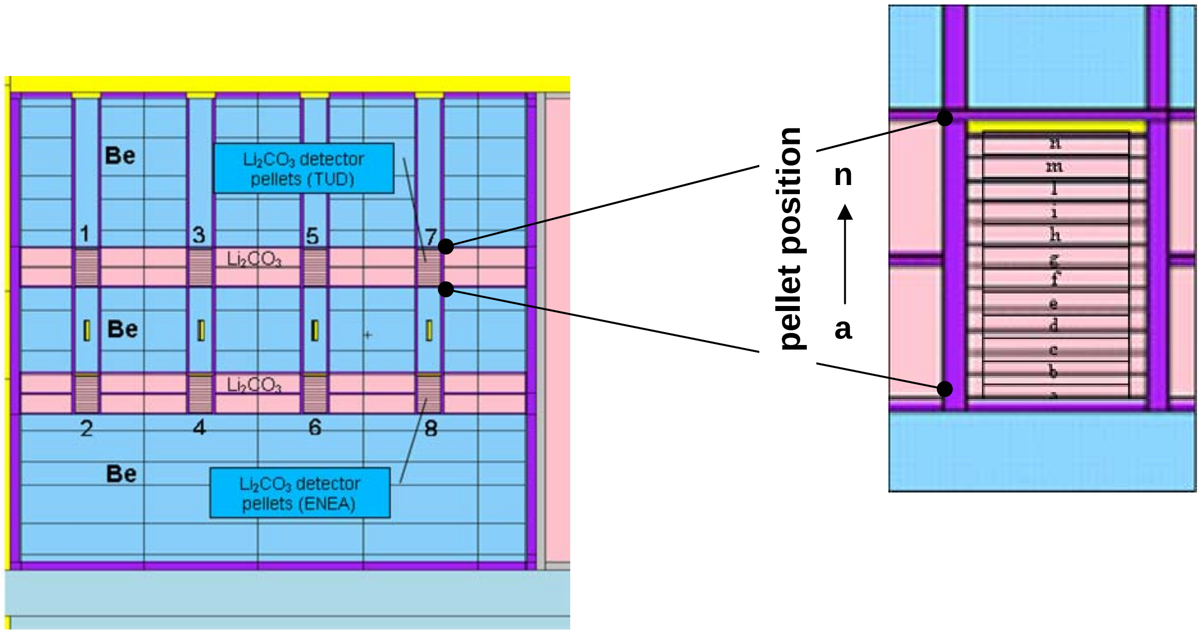

FIG. 6: MCNP model of the HCPB TBM mock-up (vertical cut through the centre of the assembly).

The Tritium generated during irradiation in a series of Li_2CO_3 pellets located at different penetration depths in the mock-up was found to be underestimated by the calculations by 5 to 10% on average independent on the nuclear data used, see Figs. 7 a, b for pellet stacks1 & 2 and 7 & 8 located in the front and the back of the assembly, respectively. The obtained results indicate that design calculations for the Tritium Breeding Ratio (TBR) of fusion power reactors employing a HCPB type breeder blanket are conservative. Thus an additional TBR margin is provided which allows compensating for potential other uncertainties.

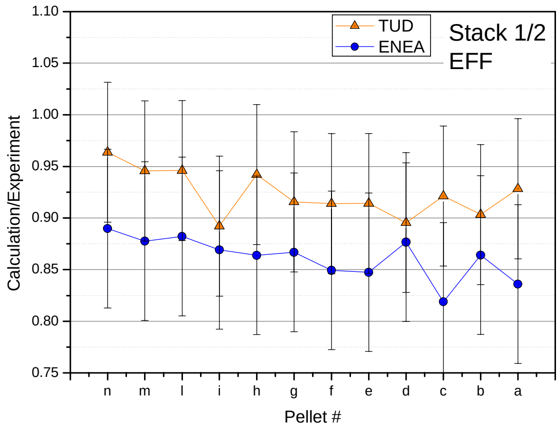

FIG. 7a: Pellet stacks 1 & 2

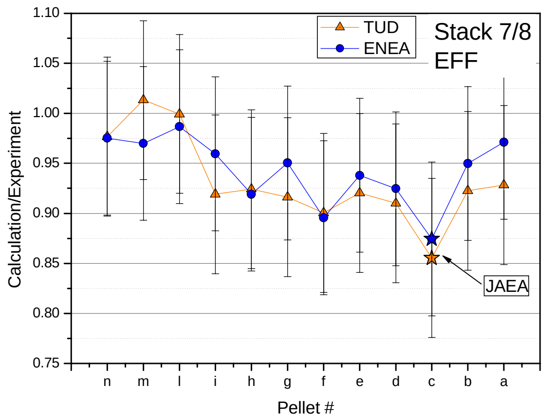

FIG. 7b: Pellet stacks 7 & 8

FIG. 7a,b: Ratios of calculated (C) and experimental (E) tritium activities measured in the pellets

6. Conclusions

Significant progress has been achieved over the past two years in making available new data evaluations satisfying the needs for neutron transport and activation calculations of the ITER device and the IFMIF intense neutron source, in developing advanced computational tools such as the CAD interface programme for the MCNP code, in extending the capabilities for Monte Carlo based calculations of sensitivities & uncertainties, and, in providing the experimental data for a breeder blanket mock-up required for validating related neutronics design calculations. Further R&D work is required though to ensure a continuous adaptation of the computational tools and data to the changing needs of the fusion programme.

Acknowledgement

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