

Advanced Neutronics Simulation Tools and Data for Fusion Applications

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Abstract. This paper reports on development works conducted at the Karlsruhe Institute of Technology (KIT) in the field of computational tools and data for fusion neutronics applications. The related R&D activities are conducted in the frame of the Power Plant Physics and Technology (PPPT) programme of EUROfusion and specific grant agreements with F4E with the objective to make available the tools and data as required for a sufficient prediction capability of the neutronic simulations performed for fusion power reactors.

1. Introduction

Neutronics simulations play an important role for the design and optimisation of the nuclear components of a fusion reactor and the related performance analyses. Suitable computational approaches, tools and data need to be available to provide nuclear responses with sufficient accuracy. This includes a suitable method for the simulation of neutron transport in complex 3D geometries, high quality nuclear cross-section data to describe the nuclear interaction processes, and, eventually, a simulation model which replicates the real 3D geometry without severe restrictions. Such requirements are satisfied with the Monte Carlo (MC) particle transport technique which can handle any complex 3D geometry and employ the nuclear cross-section data in the continuous energy representation without any severe approximation.

Key issues for reliable neutronics simulations are thus related to the reliability of the employed MC particle transport code, the quality of the nuclear cross-section data evaluations for fusion applications, and the capability to describe in the simulation the real reactor geometry with high fidelity and sufficient detail. All of these key issues are addressed in R&D activities of the European fusion programme with the objective to provide the tools and data which are required to ensure a sufficient prediction capability of the neutronic simulations.

The focus of this paper is on the computational tools developed for the high fidelity geometry representation in MC particle simulations and the provision of high quality nuclear cross-section data with uncertainty assessments. Related activities, conducted by KIT in the frame of the Power Plant Physics and Technology (PPPT) programme of EUROfusion and specific grant agreements with F4E, Barcelona, are presented including recent achievements and applications. Complementary activities conducted in these areas are also addressed.

2. Computational tools for fusion neutronics simulations

The MC particle transport technique is the most suitable method for fusion neutronics simulations since it is capable of handling complex 3D geometries like tokamaks or stellarators and employing the nuclear cross-section data in the continuous energy representation without any severe approximation. With the high performance computers available nowadays, it is even possible to provide high resolution 3D maps of nuclear responses with sufficient statistical accuracy throughout the entire geometry. MC codes suitable for fusion neutronics applications are briefly addressed in section 2.1

A key issue of faithful neutronics simulations is the capability to describe in the MC simulation the real reactor geometry with high fidelity and sufficient detail. This can be achieved with a modelling approach which ensures a true one-to-one translation of the CAD geometry, as produced for the engineering design, into the MC geometry representation. Such an approach is enabled with the McCad conversion software [1, 2] presented in section 2.2.

2.1 Monte Carlo codes for fusion neutronics applications

The Monte Carlo code MCNP with the current versions 5 and 6 [3, 4], developed by the Los Alamos National Laboratory (LANL), USA, is the standard code for fusion neutronics applications including ITER and DEMO. MCNP is very powerful in its capabilities, well validated and benchmarked, and most suitable for fusion applications. MCNP, however, is subject to US export control regulations. Several alternative MC codes have been considered for the PPPT programme [5]. The TRIPOLI-4 code [6], developed by CEA Saclay, France, was selected as most promising candidate and was accepted as analysis code for PPPT. TRIPOLI-4 is a mature code, well advanced in its functionalities, successfully validated for fusion neutronics and benchmarked against MCNP for DEMO application to [7,8]. It is thus required to provide interfaces for the TRIPOLI-4 MC code which enable access to the CAD geometry data. This issue is addressed by KIT through the McCad software development.

The open source MC codes SERPENT [9] and GEANT [10], both freely available, are also considered as long-term alternatives which still require substantial development and qualification effort for fusion neutronics applications including the adaptation to DEMO analysis needs. Related development work on these codes is not conducted within the EUROfusion programme. The McCad software, however, has been already extended to process CAD geometry data for use with GEANT, see section 2.2.3.

2.2 The CAD to MC geometry conversion tool McCad

The McCad conversion software has been developed at KIT to enable the automatic conversion of CAD models into the semi-algebraic geometry representation as utilized in MC particle transport simulations. McCad is entirely based on open-source software and libraries, which utilizes Open Cascade (OCC) as CAD kernel and the Qt4 and OpenGL libraries for the graphical user interface (GUI). CAD geometry data can be imported via neutral files (STEP/IGES), visualized with McCad's GUI, converted into Monte Carlo geometry representation and output in the syntax of the MC codes including MCNP and TRIPOLI.

The current development work on McCad is conducted within the PPPT programme of EUROfusion. The latest enhancements include improved algorithms for the decomposition of solids with the addition of splitting surfaces, a collision detecting technique based on mesh triangles, and an algorithm for the sorting of the splitting surfaces. These improvements were

verified with several test models derived from the DEMO model and were shown to result in a more efficient conversion process with a better, less complex, geometry representation. Fig. 1 illustrates the decomposition process, as enabled with McCad's new decomposition algorithm, on the example of DEMO model components.

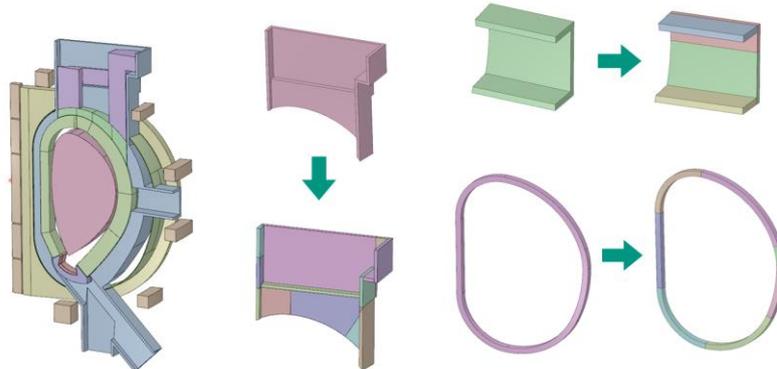


FIG. 1: Automated decomposition of DEMO model components with McCad's new decomposition algorithm

2.2.1 McCad interface for TRIPOLI-4

The McCad interface for TRIPOLI-4 has been developed only recently on the basis of the already existing conversion functionalities developed for MCNP. TRIPOLI utilizes a similar geometry description as MCNP, namely the constructive solid geometry (CSG) representation, though with different syntaxes. In MCNP, a combination of convex solids can be described directly with a variety of symbols while TRIPOLI defines each decomposed convex solid as virtual cell and then defines the combination geometry with these virtual cells. McCad creates void spaces after the conversion of material solids. In TRIPOLI, those parts of material solids colliding with void boxes also have to be defined first as virtual cell, afterwards the void spaces are defined by combination of these virtual cells. Some new classes have been thus added to McCad for the TRIPOLI file generation.

Successful verification tests have been performed for the conversion of various DEMO models. These tests included, among others, detailed comparisons of MCNP and TRIPOLI models derived from the same underlying CAD model. Recent applications of McCad's TRIPOLI interface within the PPPT programme are shown below in section 2.2.5.

2.2.2 McCad implementation on the SALOME simulation platform

The McCad software, originally developed under the Linux operation system, has been also ported to the Windows platform. This has been achieved through its implementation on the SALOME simulation platform [11]. A new Graphical User Interface (GUI), as shown in Fig. 2, was developed to this end on SALOME under Windows. The SALOME platform builds on the same graphic kernel as McCad and provides a convenient and flexible interactive graphic environment. To make McCad available on the SALOME platform, new conversion function modules including the decomposition, the void filling and the material editing have been integrated. The CAD to MC geometry conversion is thus enable just by calling the McCad conversion functions in SALOME. Fig. 2 shows a screenshot of the SALOME GUI for McCad with a torus sector model and the parameter setting window.

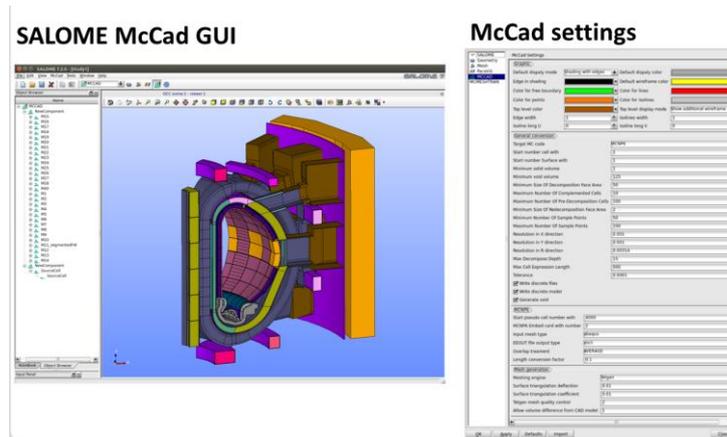


FIG. 2: McCad GUI on the SALOME simulation platform (left) and window with Mcad settings (right)

2.2.3 Advanced McCad features

As a further advanced feature, the support of the hybrid geometry modelling technique has been implemented in McCad. This technique enables to combine s CSG geometry models and models composed of tessellated solids or unstructured meshes. The converted hybrid models can be used with MCNP6 which has the capability to track particles on unstructured meshes. Fig. 3 shows an example of such a hybrid model developed for an HCPB blanket module.

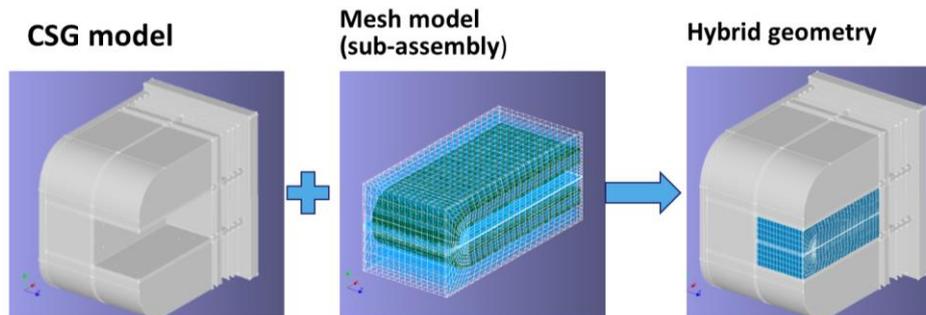


FIG. 3: Generation of hybrid geometry model for MCNP6 with McCad.

In addition, a dedicated interface has been developed for the Open Source MC code GEANT4. GEANT4 uses primitive CSG solids like boxes, spheres, and cylinder sections. A half-space based CSG solid approach was thus developed to enable the required CAD geometry conversion. The Geometry Description Markup Language (GDML) was extended to store this solid type, and the Geant4 GDML parser was enabled to process the solids. A GDML interface was developed to export the converted CAD solids. Complex CAD solids which cannot be converted are tessellated into facets and exported to GDML as tessellated solids. Successful test verifications have been performed for simple geometry set-ups. Extensive testing is underway for a full 3D ITER torus model.

McCad is conceived as open source software and is thus available without restrictions. The software package, including source code and pre-compiled binaries, is available on the GitHub platform, see <https://github.com/inr-kit/McCad>. Additional tools allow to process high resolution mesh tally data and visualize them on the CAD geometry. For coupled multi-physics analyses, involving e. g. CFD and FEM calculations, such data can be also exchanged with other codes, integrated as SALOME modules or linked via external interfaces [12, 13].

2.2.4 McCad applications

McCad is predominantly used for generating the DEMO simulations models for the various nuclear analyses performed within PPPT. The general modelling approach is to generate first a generic CAD neutronics model from the CAD Configuration Management Model (CMM). This model includes the Toroidal Field Coil (TFC), vacuum vessel (VV), divertor, blanket segment box, vessel ports, and plasma chamber, represented in a single torus sector with envelopes. All components are thus described by their bounding surfaces (“envelopes”) without any internal structure specified. This model is converted to analysis models for the MC simulation codes with McCad and serves as basis for the adaptation to specific tasks.

Such specific tasks are, among others, design analyses for the development of different breeder blanket concepts for DEMO. Accordingly, specific models are derived from the generic DEMO model by integrating blanket modules of the different breeder blanket concepts. Thus specific DEMO breeder blanket models are generated which are consistent with the DEMO baseline and the specific engineering blanket design. Figs. 3 and 4 illustrate this process on the example of DEMO variants with a Helium-Cooled Pebble Bed (HCPB) and a Helium-Cooled Lithium Lead (HCLL) breeder blanket, prepared for the MCNP and TRIPOLI 4 MC codes, respectively.

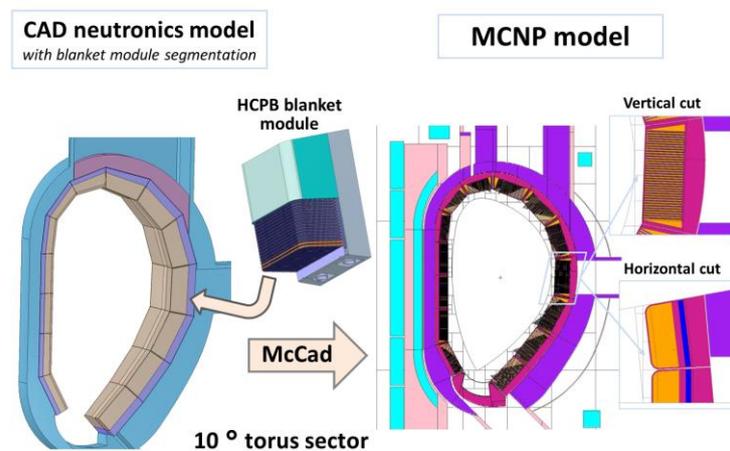


FIG. 4: Generation of an MCNP simulation model of DEMO with HCPB blanket modules

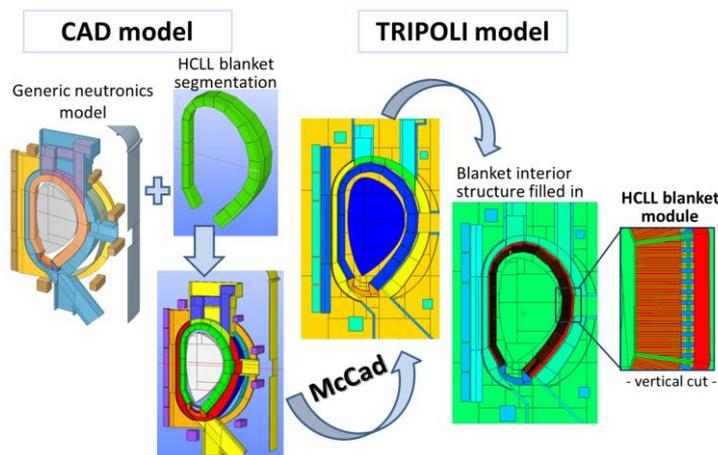


FIG. 5: Generation of a TRIPOLI-4 analysis model of DEMO with HCLL blanket using McCad's windows version on the SALOME platform

3. Nuclear data for fusion applications

To satisfy the needs for high quality nuclear data, a dedicated programme on Nuclear Data Development (NDD) is conducted with the support of F4E. The related activities include the evaluation and validation of nuclear cross-sections, the development/extension of codes and software tools for nuclear model calculations and sensitivity/uncertainty assessments. After passing a thorough benchmarking and validation process, the cross-section data evaluations are eventually fed into the Joint Evaluated Fusion File (JEFF), maintained by the NEA Data Bank, Paris, France. Special data libraries are developed for activation/transmutation, gas production and displacement damage calculations.

3.1 Neutron cross-section data for general purpose calculations

Such cross-section data evaluation are required for transport calculations and thus include all reactions cross-sections as function of the neutron energy as well as secondary angle and energy distributions. KIT's recent evaluation efforts were on the neutron cross-sections of $^{63,65}\text{Cu}$ and $^{90,91,92,94,96}\text{Zr}$. The evaluations are based on nuclear model calculations with the TALYS code [14] including an improved description of the pre-equilibrium emission of particles with a modified version of the geometry depend hybrid (GDH) model. This results in a better reproduction of the neutron emission spectra as shown in Fig. 6 for Cu and Zr. This is essential for an accurate simulation of the neutron transport through materials such as the CuCrZr alloy used as heat sink material for divertors. The evaluated data were tested against available benchmark experiments such as the one performed at the Frascati Neutron Generator [15] on a Cu assembly. Good agreement is obtained for most reaction rates as shown in Fig. 7.

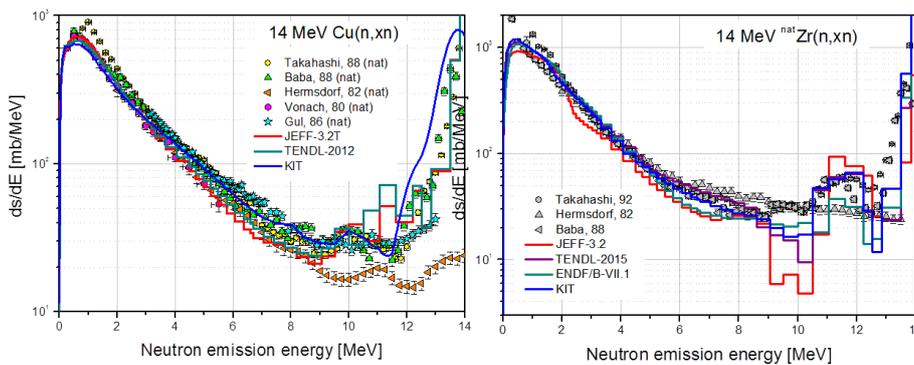


FIG. 6: Neutron emission spectra for natural Cu (left) and Zr (right)

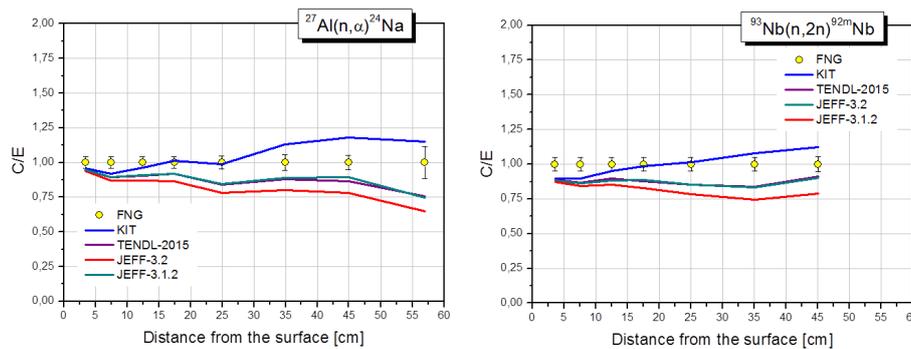


FIG. 7: C/E (calculation/experiment) ratios of the $^{27}\text{Al}(n,\alpha)^{24}\text{Na}$ (left) and $^{93}\text{Nb}(n,2n)^{92m}\text{Nb}$ (right) reaction rates measured in the FNG copper benchmark [15].

3.2 Damage displacement and gas production data

Displacement damage cross-section data were evaluated for the Eurofer and SS-316 steels using advanced modelling approaches which take into account Binary Collision (BC) and Molecular Dynamics (MD) simulation results for the calculation of the number of lattice defects. This results in significantly lower dpa cross-sections as compared to the standard NRT damage model approach, see Fig. 8 (left side). Related cross-section data files were prepared for the two steels and made available through the IAEA, Vienna.

In addition to the displacement damage, the production of gases like hydrogen and helium strongly affects the behaviour of materials under irradiation. A systematic evaluation of gas production cross-sections was performed for nuclides from $Z=12$ to 83. This evaluation is based on available experimental data, nuclear model calculations and systematics. Fig. 8 (right side) shows, as example, the helium gas production cross-section evaluated for Cr compared to available experimental data.

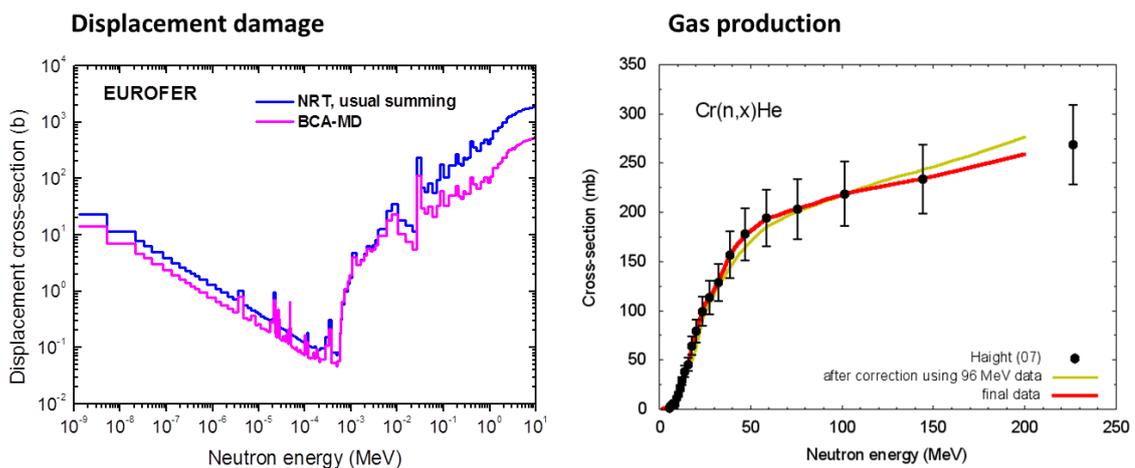


FIG. 8: Evaluated displacement damage and helium gas production cross-sections for Eurofer (left) and chromium (right), respectively.

3.3 TBR sensitivity/uncertainty analysis for DEMO

The issue of sensitivity/uncertainty (S/U) assessments, including related tool developments and application analyses, is also addressed within the NDD activities. The aim is to enable the identification of important reactions for relevant responses, and quantify the associated uncertainties. To this end the MCNP based sensitivity code MCSSEN [16] has been developed. MCSSEN is a local extension to MCNP with the capability to calculate sensitivities by the point detector and the track length estimator. This enables the efficient calculation of sensitivities for nuclear responses in an arbitrary 3D configuration. Thus the real 3D model of a fusion reactor, as used in design analyses, can be employed. On this basis, uncertainty estimates can be obtained for a real reactor geometry without approximations. This capability was tested for an HCPB DEMO model developed within the PPPT programme.

The sensitivity and uncertainty of the tritium breeding ratio (TBR) were calculated for the reactions on the major nuclides including ^1H , ^6Li , ^7Li , ^9Be , ^{16}O , $^{28,29,30}\text{Si}$, $^{54,56}\text{Fe}$, ^{52}Cr , ^{58}Ni , and $^{182,183,184,186}\text{W}$. The related covariance data were taken from JEFF-3.2 whenever available, from FENDL-2.1 for ^7Li , from EFF-3 for ^9Be and from JENDL-3.2 for ^{16}O . In addition, covariance data from the TENDL-2014 library were also used. The TBR was shown to be pre-dominantly sensitive to the ^{16}O data, followed by $^{6,7}\text{Li}$, ^{28}Si , ^9Be and ^{56}Fe . An overall

uncertainty of $\pm 3.2\%$ was obtained for the TBR when using JEFF-3.2 covariance data with the mentioned additions. The uncertainty is dominated by the uncertainties of the ^{16}O , ^6Li and ^7Li cross-sections. When using TENDL-2014, the uncertainty estimate increases to ca. $\pm 10\%$.

4. Conclusions

Development works conducted at KIT in the field of computational tools and nuclear data for fusion neutronics were presented. Significant progress was achieved for the high fidelity geometry representation in MC particle transport simulations through the translation of CAD geometry data for the MCNP, TRIPOLI and GEANT4 Monte Carlo codes with extended capabilities of the McCad conversion software. Application examples were shown on various DEMO models demonstrating the relevance of such capabilities for the PPPT programme. Nuclear data evaluations relevant to fusion technology were provided for neutron transport applications, displacement and gas production calculations as well as uncertainty assessments.

Acknowledgments

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References:

- [1] LU, L., FISCHER, U., PERESLAVTSEV, P., "Improved algorithms and advanced features of the CAD to MC conversion tool McCad", *Fus. Eng. Des.* 89 (2014) 1885-1888
- [2] LU, L., FISCHER, U., QIU, Y., PERESLAVTSEV, P., "The CAD to MC geometry conversion tool McCad: Recent advancements and applications", *Mathematics and Computations (M&C)*, Nashville, USA, April 19-23, 2015, Proc. on CD-ROM, LaGrange Park, Ill. : ANS (2015)
- [3] X-5 Monte Carlo Team, "MCNP – A general Monte Carlo N-particle Transport Code, Version 5," LA-UR-03-1987, Los Alamos National Laboratory (April, 24, 2003).
- [4] MCNP6 Users Manual - Code Version 6.1.1beta, LA-CP-14-00745 (June 2014)
- [5] FISCHER, U., et al., "Neutronic analyses and tools development efforts in the European DEMO programme", *Fus. Eng. and Des.* 89 (2014), 1880-1884.
- [6] TRIPOLI-4 PROJECT TEAM, "TRIPOLI-4 version 8 User Guide", CEA-R-6316 (2013).
- [7] FAUSSER, C., GABRIEL, F., "TRIPOLI-4 validation for fusion blankets design", CEA report SERMA/10-4993, 2010
- [8] JABOULAY, J.-C., et al., "Comparison over the Nuclear Analysis of the HCLL blanket for the European DEMO", *Fus. Eng. and Des.* 109-111(2016), 365-370
- [9] LEPPÄNEN, J., <http://montecarlo.vtt.fi/index.htm>
- [10] GEANT-4 Collaboration, <http://geant4.cern.ch/>
- [11] <http://www.salome-platform.org>
- [12] QIU, Y., LU, L., FISCHER, U., "An advanced MC modelling and multi-physics coupling system for fusion applications", *Mathematics and Computations (M&C)*, Nashville, USA, April 19-23, 2015, Proc. on CD-ROM, LaGrange Park, Ill. : ANS (2015)
- [13] QIU, Y., "Development of a coupling approach for multi-physics analyses of fusion reactors", PhD thesis, Karlsruhe Institute of Technology, May 2016.
- [14] KONING, A. J., ROCHMAN, D., "Modern nuclear data evaluation with the TALYS code system", *Nuclear Data Sheets* 113 (2012) 2841
- [15] ANGELONE, M., et. al, "Copper benchmark experiment at the Frascati Neutron Generator for nuclear data validation", *Fus. Eng. and Des.* 109-111 (2016) 843
- [16] PEREL, R. L., "Upgrading of the MCSSEN sensitivity software to comply with the current standard of the MCNP-5 Monte Carlo code", Karlsruhe Institute of Technology (KIT), internal report, November 2014.