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André Häußler[a], Ulrich Fischer[a], Felix Warmer[b]

[a]Karlsruhe Institute of Technology (KIT), Institute for Neutron Physics and Reactor Technology (INR), 76344 Eggenstein-Leopoldshafen, Germany
[b]Max Planck Institute for Plasma Physics (IPP), 17491 Greifswald, Germany

Three different approaches were investigated for the use of CAD models with Monte Carlo transport simulations of a simplified stellarator type verification geometry. These include the traditional Constructive Solid Geometry (CSG) approach with the geometry translated into Monte Carlo representation, the use of Unstructured Mesh (UM) geometry as available with MCNP6, and the direct particle tracking technique of DAGMC. The three methods were shown to be both applicable and suitable to represent the verification geometry and provide comparable results. With regards to the later application to a real stellarator geometry, the DAGMC and the UM approaches are preferred over the CSG approach due to the inherent limitations of the latter.

Keywords: STELLARATOR, CAD, MCNP, DAGMC, NEUTRONICS, VERIFICATION

1. Introduction

The Helical-Axis Advanced Stellarator (HELIAS) is a conceptual design of a fusion power reactor proposed by the Institute for Plasma Physics (IPP) in Greifswald, Germany. HELIAS-5B is a specific 5-field-period concept using the Deuterium-Tritium fusion reaction with a fusion power of 3000 MW [1]. A thorough neutronic design analysis has to be performed for this stellarator in order to provide the input required for the reactor design.

A stellarator confines the hot plasma with external magnetic fields only produced by non-planar shaped modular field coils. The use of specific non-planar shaped modular field coils is necessary to generate the rotational transform of the magnetic field in the plasma chamber. This type of fusion reactor represents a challenging task for the design and maintenance of technological components such as the breeder blanket and the radiation shield as outlined in figure 1.
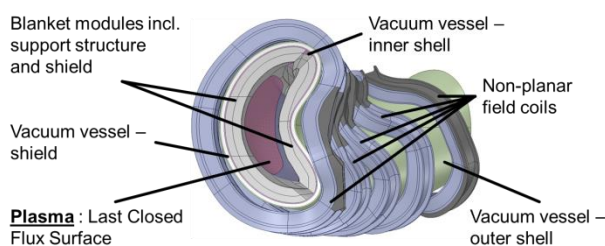

Fig. 1: HELIAS-5B CAD model including material layers and last closed flux surface

The standard approach to develop geometry models for neutronics design analysis is to use computer aided design (CAD). The developed models are usually not directly applicable for Monte Carlo (MC) particle transport codes and need preprocessing with regard to the geometrical simplification and adaption to the requirements of neutronic simulations including the decomposition of complex CAD models.

The CAD model of the HELIAS reactor is very complex and contains mostly spline surfaces which are commonly used in CAD geometry. Spline surfaces are higher order surfaces and not directly applicable in MC simulations. This makes a translation approach for CAD to MC geometry necessary which is able to take spline surfaces into account in the processing of the models.

The purpose of this paper is to investigate the feasibility and suitability of three different CAD to MC geometry translation approaches on the example of a dedicated verification geometry model. The comparison of the three methods allows concluding on their applicability to design analyses of a stellarator type reactor.

2. Methodology

Three different approaches to generate a CAD based MC geometry will be discussed in this paper. First, the translation approach with KIT's CAD to MC conversion tool McCad [3]; second, the unstructured mesh geometry description approach [4]; third, the direct usage of CAD geometry in MC codes with DAGMC (DAG = direct accelerated geometry) [5].

The first approach uses McCad to translate the CAD geometry into constructive solid geometry (CSG) which most MC particle transport codes use as geometry representation. This is the standard geometry translation approach for fusion neutronic calculations and needs to be investigated for the application to stellarator reactors. In the CSG description mainly first and second order surfaces are allowed, e.g. planes and cylinder as adopted by the MC particle transport codes. Spline surfaces are not supported and McCad does not translate them. For a complex geometry like the stellarator, the CSG method, without CAD model simplification and modification, is not useable. Nevertheless, this MC geometry description

is the best verified and validated method of all three investigated methods.

MCNP6 includes as a new feature the capability to use an unstructured mesh (UM) geometry representation in the particle tracking simulation. This feature enables the possibility to construct an UM model which allows using all types of surface descriptions in the CAD model. This leads to the advantage of this method that very complex geometries can be handled in MC simulations without profound simplification or decomposition. The limitations are mainly given by MCNP6, because only one specific mesh type can be handled in one simulation at the same time. In this work, ANSYS Workbench 16.2 [5] was used as meshing tool to generate the unstructured mesh geometry. It is thus possible to adapt the generated mesh to the limitations of MCNP6.

As third method the DAGMC approach for the direct use of CAD geometry in the MC transport simulation was applied. DAGMC adaptations to different MC radiation transport codes are available. For this work, the DAGMC patch for MCNP was applied. DAGMC converts the CAD geometry into facetted solids for the tracking of particles. The tracking algorithm implemented in DAGMC is based on the established ray-tracing technique. With this technique it is possible to perform simple calculations to determine the next surface boundary, depending on the particle position and its movement trajectory [6]. DAGMC can solve analytically a number of lower order surfaces, but higher order surfaces require iterative numerical root-finding approaches which are implemented in DAGMC with a number of acceleration techniques and approximations [6]. This ensures that the method can be efficiently used for high order spline surfaces. The CAD geometry is prepared with Trelis 16 [7] to ensure that all bodies and surfaces are preprocessed and facetted in the correct way for the use with DAGMC.

MCNP is a general-purpose Monte Carlo N-Particle code which is used worldwide, very well validated and applied in the fields of fission, fusion and accelerator calculations. In this work MCNP6.1.1beta [8] was used for CSG and UM calculations. For the use with DAGMC calculations it is important to apply a special patch to MCNP. The latest version which is supported by DAGMC is MCNP5.1.60 [9] thus was used for all DAGMC calculations.

3. CAD verification geometry development

The methods discussed for creating a suitable MC particle transport geometry need to be tested and verified. To this end, a dedicated CAD verification geometry was designed which fits into all limitations of the discussed methods. In fact, the traditional CAD to MCNP translation approach gives the boundary conditions for the CAD geometry, because the CSG description has the most limitations.

In the verification geometry only cylinders and planes are included which represent the boundary conditions for the CSG geometry with first- and second-order surfaces. The verification geometry is based on a bean-shaped cross-section of the stellarator as shown in figure 2. It has a total height of about 1030 cm, a width at the equatorial plane of about 480 cm and a depth of 100 cm.
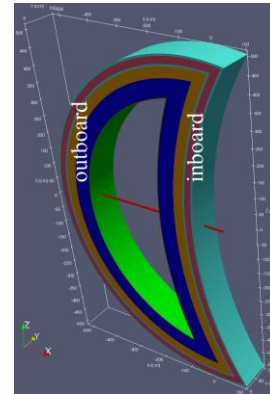

Fig. 2: Verification geometry with layers; the red line indicates the tally locations used for the verification calculations

The radial build of the verification geometry along the red line shown in figure 2 is given in table 1.

Tab. 1: Radial build of the verification geometry at the mid-plane

Thickness [cm]	Component / material
0.2	Tungsten Armor
2.5	First Wall
50	Breeding Zone
30	Back Support Structure
6.0	Inner Vacuum Vessel
20	Vacuum Vessel Shield
6.0	Outer Vacuum Vessel

These layers represent the first preliminary geometry requirements for the HELIAS-5B. Each layer contains a homogenized material mixture. For the breeder zone the helium cooled pebble bed (HCPB) blanket concept [10] is assumed as one option to breed tritium in the stellarator. Here its homogenized material composition is used. The back support structure is a mixture of the back plate, made of low activation steel, and the manifold. It thus contains mostly steel with a lower density to take the cooling channels into account. As shielding layer inside the vacuum vessel, a mixture of 60 % water and 40 % stainless steel is used.

A volumetric 14.1 MeV neutron source is included inside the plasma chamber with a length of 100 cm in y direction to fill up the space in the geometry. It contains in total four different neutron emission probability areas to represent the similar behavior as the plasma source of the HELIAS-5B [11]. Reflecting boundary conditions are set on both open sides of the verification geometry.

4. Computation and Results

The CAD verification geometry was processed in three different ways to generate a suitable MCNP geometry description. This can be seen in figure 3.
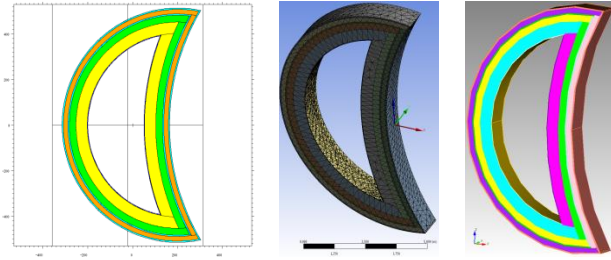

Fig. 3: Verification geometry shown in CSG, in Unstructured Mesh and in DAGMC representation

In the unstructured mesh geometry, only a limited number of standard tallies in MCNP6 are supported. These are cell tallies for "Flux averaged over a cell" and "Energy deposition averaged over a cell" [4]. In addition, two different mesh tallies were superimposed over the geometry during the simulations. One mesh tally covers the whole verification geometry with a resolution of $1 \times 1 \times 1$ cm^3. The other mesh tally is parallel to the x axis and crosses the y axis at 50 cm and the z axis at 0 cm. It has also a resolution of $1 \times 1 \times 1$ cm^3 and is indicated as red line in figure 2.

To get tally results for all single material zones, the cell tallies were applied on all of the 14 solids of the geometry. In order to find differences or mismatches between the investigated methods the tally results are compared. All calculations were performed at the KIT Institutscluster II (IC2) [12].

Significant differences in the computational time were obtained. The CSG method needed ~29000 CPU minutes, UM ~57000 CPU minutes and DAGMC ~58000 CPU minutes. Thus there is a factor of two higher computational time of UM and DAGMC geometry description compared to the calculations with the traditional CSG geometry.

In figure 4 the neutron flux and the corresponding error in the whole verification geometry is shown. It is a cut along the xz plane at y = 50 cm.
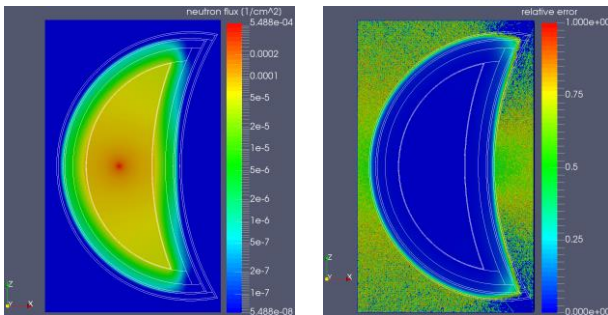

Fig. 4: Neutron flux per history and corresponding relative error in the verification geometry calculated with the CSG method

The distribution of the neutron flux is clearly seen and also its attenuation in direction from the plasma chamber to the vacuum vessel. In the regions far away from the neutron source the neutron flux is lower and the relative error higher which is a normal behavior in neutronics simulation.

The same behavior can be seen in figure 5 and figure 6. Both figures show the neutron flux along the red line indicated in figure 2, one at the outboard (Fig. 5) and one at the inboard (Fig. 6).
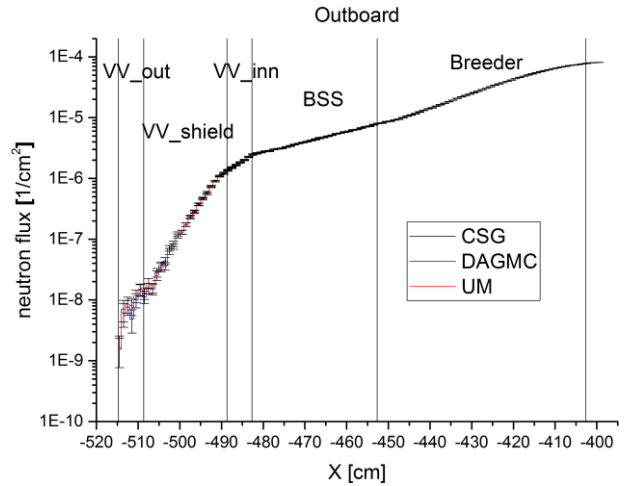

Fig. 5: Neutron flux per history at the outboard side of the verification geometry
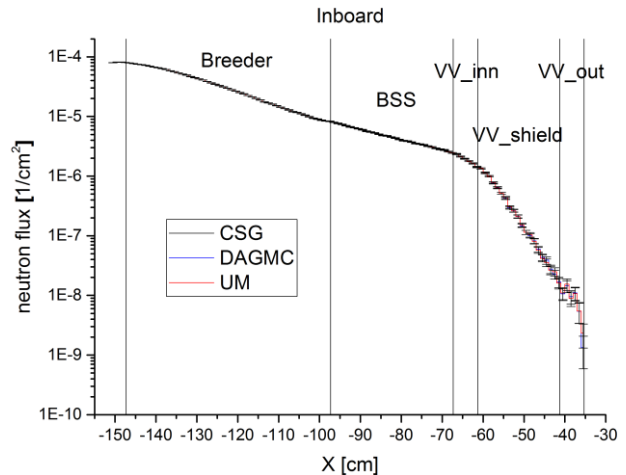

Fig. 6: Neutron flux per history at the inboard side of the verification geometry

Figure 5 and 6 show that the neutron flux is decreasing from the plasma side to the vacuum vessel. The profile is related to the radial build (layer thickness and the material composition) as shown above.

It is noted that all three investigated geometry translation methods give identical results within the statistical uncertainty. The small differences of DAGMC in the vacuum vessel outer layer are related to MCNP

which can be reproduced by running the CSG geometry with MCNP5.

The results for the cell tallies show basically the same behavior with nearly identical results between all three investigated methods. The largest difference can be detected in the tungsten layer in the outboard between CSG and UM method. For the flux tally 1.75 % and for the heating tally 1.58 % was found. All other differences between the methods are much smaller and negligible with respect to the corresponding relative error.

All three methods seem thus to be suitable for neutronics design analysis of a stellarator. The CSG method, however, has the drawback that no spline surfaces are supported in the geometry description which requires manually simplification and decomposition of the CAD model. This is a long lasting and error prone process, because no automation so far is applicable for this procedure. The UM method is suitable, but it has a strict limitation of the supported tallies available currently with MCNP6. It is thus considered as a current additional approach, but not as the preferred method for calculations for the stellarator. DAGMC has the drawback that a lot of dependencies to different software suits are needed during the installation process which makes it complicate to install and run. The outstanding features of DAGMC are first, that it can handle very complex geometries and second, that all tallies from MCNP are supported.

5. Conclusion and outlook

Three different geometry representation approaches for MC based nuclear analyses were investigated and successfully tested on a simplified geometry model. All three approaches give comparable results within statistical uncertainty despite significant differences in the geometry set-up.

The investigated methods can be used for neutronic design analyses of HELIAS based on a suitable CAD model. The CSG method, however, has inherent limitations and is thus not the preferred method. The DAGMC method is preferred because it can handle the complex spline based geometry and it supports all tallies from MCNP.

Acknowledgments

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