Monte Carlo with optimized 3D geometries

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Methodology

Monte Carlo calculations for applications related to particle transport through matter are performed using different packages, including MCNP [1], FLUKA [2, 3] and PHITS [4].

Large portion of time in such simulations is usually spent on building geometric models (especially when modelling complex facilities with thousands of components).

In these packages the regions are described by Boolean functions with surfaces as literals:

```
287 0            270 −276 −665 −314 316 312 274
288 5  0.0582256 ( −268 : 269 : −270 : 271 ) −157 156 −155 154 −311 310
289 73 0.0844385 270 −276 ( −319 : −315 : −280 ) ( −318 : 314 : −280 )
                 ( −317 : −315 : 665 ) ( −316 : 314 : 665 ) −164 274 −313 312
```

Managing and optimising complex models in such format can be difficult, therefore instead of editing the input files manually, we do it with a home-built CombLayer tool [5]. It allows to describe Constructive Solid Geometry in object-oriented approach, so that the whole model is made of C++ objects.

The purpose of CombLayer is to easily and rapidly build complex geometric models which are fast to run in MCNP like Monte-Carlo codes.

It achieves this by a two factor Boolean optimisation to minimise number of literals (surfaces). In intersections it removes unnecessary surfaces and allows the cells to be split or merged as needed without Monte Carlo run-time cost.

The program uses modifiable plug and play component modules to produce a highly parametric space-filling geometry models described by quadratic surfaces. Each module is described in a local coordinate system and then can be inserted anywhere, and with any orientation.

The code exports models for the MCNP/FLUKA/PHITS nuclear simulation programs (Figs. 1 and 2) as well as POV-Ray [6] (Fig. 6) and VTK. The internal tracking system allows geometry validation and variance reduction.

Geometry simulation methodology is similar to GEANT 4 in that component types are defined in a class and used in multiple locations but the output is optimized for a Constructive Solid Geometry system.

Possibility to export models in different nuclear simulation formats allows to check results with different codes and use the most suitable tool for the particular purpose.

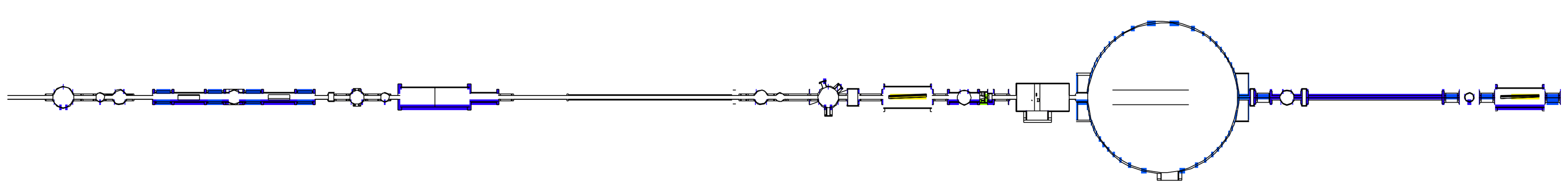

Figure 1: Part of MAX IV SoftiMAX beam line displayed with MCNP

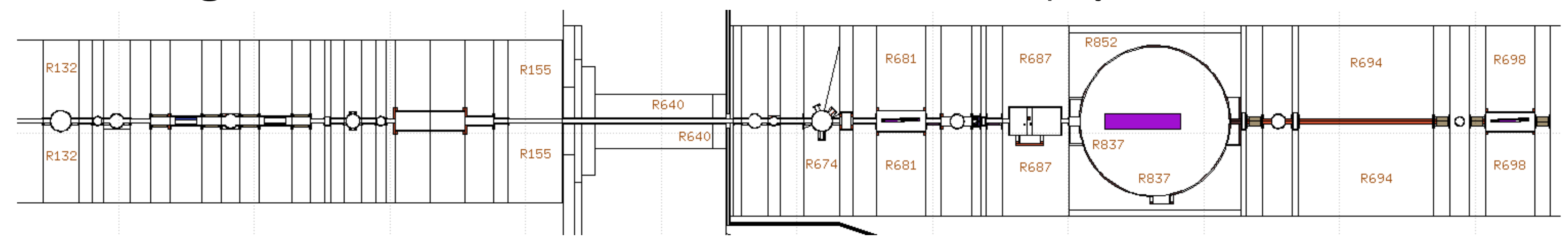

Figure 2: The same model displayed with FLUKA. Note that complex regions must be split to allow FLUKA to calculate disjunctive normal forms.

Applications

This section covers some aspects of our experience using CombLayer at the European Spallation Source and MAX IV facilities located in Lund, Sweden.

Radiation shielding

Figures 1, 2 and 6 show the same part of the MAX IV soft x-ray beamline SoftiMAX visualised by different packages.

In the shielding calculations, one has to consider lots of scenarios with different geometric configurations as well as optimize thicknesses and materials of various shielding sections.

Since the models in CombLayer are fully parameterised, this requires nothing more than changing the corresponding variables either as command line arguments or .xml file entries.

Neutronics

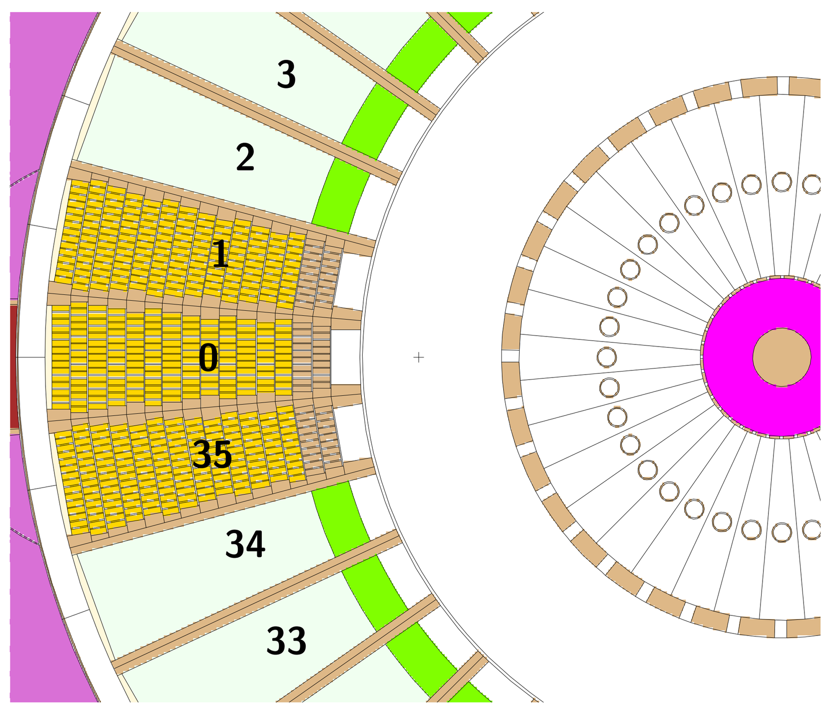

Figure 3: Detail of ESS spallation target

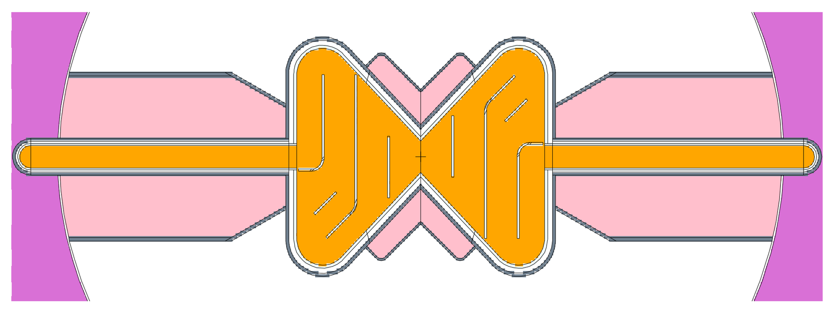

Figure 4: ESS type 1 moderator

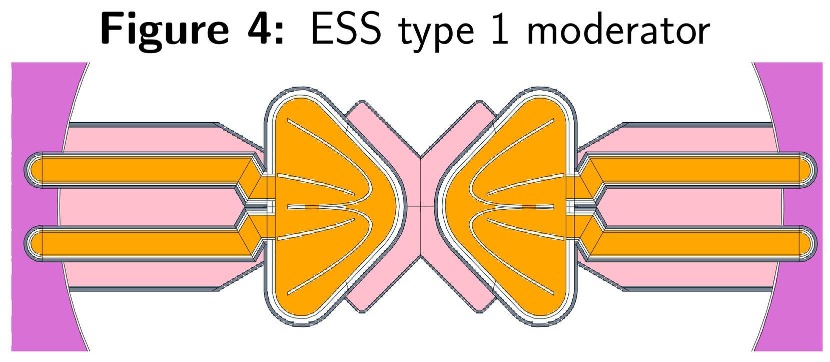

Figure 5: ESS type 2 moderator

Figures 3 – 5 illustrate models of ESS spallation target and neutron moderators.

The cylindrical spallation target consists of 36 sectors (numbered Fig. 3), each sector is made of ∼200 bricks of Tungsten.

In CombLayer, each sector is an instance of a class, so the target consists of 36 copies of the same object. However, due to calculation performance reasons, it's reasonable to model individual Tungsten bricks as homogenised material (as in sectors 2, 3, 33 and 34) and use detailed geometry with bricks only when needed (sectors 0, 1 and 35). This is achieved just by changing a single variable:

```
<variable name="TargetSector1BricksActive" type="int">1</variable>
```

In order to maximize neutron production, both target and moderator dimensions, positions, orientations and materials should have been optimized. For example, different configurations of moderators were studied (two of them are shown in Fig. 4 and 5).

Replacing one moderator configuration with another as well as changing dimensions is easily achieved with these lines:

```
<variable name="ModeratorType" type="std::string">BF1</variable>
<variable name="ModeratorWallThickness" type="float">10.0</variable>
```

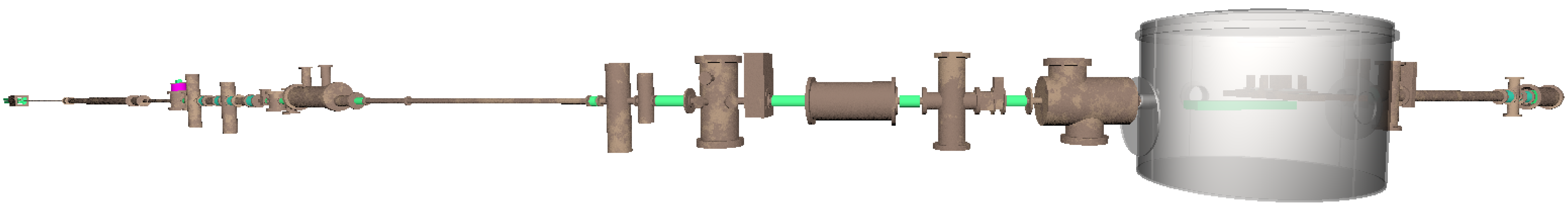

Figure 6: Part of MAX IV SoftiMAX beam line rendered with POV-Ray

References

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