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# SERPENT validation and optimization with mesh adaptive search on stereolithography geometry models ☆

Alberto Talamo [a,*], Yousry Gohar [a], J. Leppänen [b]

[a] Nuclear Engineering Division, Argonne National Laboratory, 9700 S Cass Ave., Lemont, IL 60439, USA
[b] VTT Technical Research Centre, P.O. Box 1000, FI-02044 VTT, Finland

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ABSTRACT

The SERPENT Monte Carlo code has the unique capability to simulate neutron and gamma transport using a stereolithography (STL) geometry. The STL geometry can model irregular complex geometries often encountered, for example, in research reactors. This geometry type can be used in combination with an unstructured mesh-based interface to couple SERPENT to OpenFOAM for CFD analyses. The STL file format also allows printing the geometry model with 3D printers. This work validates SERPENT simulations based on the STL geometry using the GIACINT critical experimental facility and the YALINA Thermal subcritical experimental facility. The results and performances of SERPENT have been compared with those of the well-known MCNP code. Finally, SERPENT computing time has been significantly reduced by using its mesh adaptive search algorithm, which has been introduced to optimize simulations based on the stereolithography STL geometry, and a hybrid modeling that mixes combinatorial and STL geometries. In this work, the STL geometry model of SERPENT involved the use of multiple software and programming languages, including: CUBIT, PYTHON, C, and MATLAB.

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## 1. Introduction

Monte Carlo modeling of nuclear reactors has the benefit of avoiding the spatial homogenization and the energy-angle discretization, which introduce approximations. Generally, Monte Carlo codes use different volume primitives to model any arbitrary three-dimensional geometry. The volume primitives are bounded by planes, spheres, cylinders, boxes, hexagons, ellipsoids, cones, tori, or arbitrary polyhedrons surfaces. The Monte Carlo model of the nuclear reactor is constructed using these volume primitives by combinatorial geometry; more precisely, arbitrary volumes are formed from the intersections, unions, or complements of primitive volumes or universes. A universe is a piece of geometry that has its own coordinates system and that fills another geometry region; it is the equivalent of a *part* in Computer-Aided Design (CAD) models for mechanical and thermal-hydraulics calculations. Universes are nested one inside another and are often used to model lattices. CAD models do not have any lattice capability. The Monte Carlo combinatorial geometry modeling described above has some limitation, for instance, helical cruciform fuel rods (Shirvan and Kazimi, 2012) cannot be modeled.

SERPENT is a general purpose neutron and photon transport Monte Carlo code developed since 2004 at VTT Technical Research Centre of Finland (Leppänen et al., 2015). This Monte Carlo code offers the possibility to model a reactor core either by using the traditional combinatorial geometry previously discussed and used by the worldwide used MCNP Monte Carlo code (Pelowitz et al., 2014), or by using a stereolithography (STL) geometry (Leppänen and Kaltiaisenaho, 2016). This latter feature is unique of the SERPENT code. The MCNP code has been developed at Los Alamos National Laboratory since 1957.

In the STL geometry, volumes are defined by the union of triangular surfaces (facets), as described in detail in Section 2. Both combinatorial and STL geometries allow using universes. The STL geometry offers unique benefits, including:

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* Corresponding author.
*E-mail address:* alby@anl.gov (A. Talamo).

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1) the CAD geometry model of the reactor or any *part* of the reactor can be directly imported in SERPENT;
2) the neutronics calculation can be easily coupled to OpenFOAM thermal-hydraulics calculation using a multi-physics interface based on an unstructured mesh that is constructed using the same CAD model (Aufiero et al., 2015; Leppänen et al., 2014);
3) the reactor model can be printed by 3D printers;
4) any type of geometry can be modeled, including helical cruciform fuel rods (as discussed in Section 7).

This study validates the SERPENT STL geometry computations with the experiments performed at the GIACINT (Talamo et al., 2014, 2016a, 2017a) (Sections 4 and 5) and YALINA Thermal (Talamo and Gohar, 2015; Talamo et al., 2016b) (Sections 3 and 5) facilities of Belarus. The parameters of SERPENT input have been optimized to reduce the computing time by the mesh adaptive search algorithm (Talamo et al., 2016b). SERPENT results and performances have also been compared with those of MCNP; both Monte Carlo codes used the ENDF/B-7.0 nuclear data library. Obviously, a computational model based on combinatorial geometry runs faster than one based on the STL geometry. Consequently, using a hybrid model can significantly reduce the computing time relative to a pure STL geometry model (as discussed in Section 6). In an optimized hybrid model, the complicated parts of the facility are modeled using the STL geometry, whereas the simple parts are modeled using combinatorial geometry and lattices.

## 2. SERPENT STL geometry modeling

A nuclear reactor CAD geometry can be created by the CUBIT software (CUBIT Toolkit, 2017), which is a geometry and mesh generation toolkit. In a CAD geometry model, a *body* is defined by the union of several volumes. CUBIT has the capability to export the CAD geometry to a STL file. In this file, each *body* (volume) is defined by the union of triangular surfaces (facets) without any information on materials data. The typical content of a STL file is:

```
solid Body_158
    facet normal -9.999247e-001 1.227134e-002 0.000000e+000
    outer loop
        vertex 1.062500e+000 1.385641e+001 2.500000e+001
        vertex 1.062662e+000 1.386960e+001 2.500000e+001
        vertex 1.062662e+000 1.386960e+001 -2.500000e+001
    endloop
    endfacet
    facet normal -9.999247e-001 1.227134e-002 0.000000e+000
    outer loop
        vertex 1.062500e+000 1.385641e+001 -2.500000e+001
        vertex 1.062500e+000 1.385641e+001 2.500000e+001
        vertex 1.062662e+000 1.386960e+001 -2.500000e+001
    endloop
    endfacet
    facet normal -9.999247e-001 -1.227134e-002 0.000000e+000
    outer loop
        vertex 1.062500e+000 1.385641e+001 -2.500000e+001
        vertex 1.062662e+000 1.384322e+001 2.500000e+001
        vertex 1.062500e+000 1.385641e+001 2.500000e+001
    endloop
    endfacet
    ....
    ....
    ....
endsolid Body_158
solid Body_159
    ....
    ....
    ....
endsolid Body_159
```

The above example defines *bodies* (volumes) #158 and #159 and lists the vertexes of the triangular surfaces for body #158 and their associated normal vectors. In the STL geometry model, the whole nuclear reactor geometry is defined by the sequence of *solid* and *endsolid* sections. In the STL file, each *body* of the geometry must have a *solid* and *endsolid* section. The precision of the STL geometry, relative to the CAD geometry, depends on the total number of triangular surfaces (facets). Clearly, more triangular surfaces provide a better representation of the CAD (real) geometry, especially when the real volumes have non-planar boundaries. Consequently, the accuracy of the STL geometry, relative to the CAD geometry, depends on the STL *feature angle*, which is set in CUBIT (since release 14.1) before the STL file exporting process. This angle is formed by two tangents starting from two consecutive vertexes (of a facet) on a curve of the CAD (real) geometry. A smaller *feature angle* implies: 1) a larger STL geometry file with more triangular surfaces; 2) a longer SERPENT computing time; 3) a higher precision in SERPENT results. CUBIT and any CAD modeling do not have lattice capability; consequently, MATLAB scripts have been used to write the CUBIT input lines that describe a lattice of fuel assemblies starting from one unit cell of the lattice.